Study of Soot Production for Double Injections of n-Dodecane in CI Engine-like Conditions

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Abstract

Soot production mechanism in multiple injections is complex since it involves its dependence on turbulent interactions of constituting injections and their combustion progress. A concise study was performed in a constant-volume combustion vessel by considering a double injection scheme of 0.3 ms pilot injection, 0.5 ms dwell time and 1.2 ms main injection (nomenclature: 0.3/0.5/1.2 ms) with n-dodecane as fuel and replicating the thermodynamic operating condition of a compression ignition (CI) engine. Experimental ambient temperature variations of 900 K and 800 K were performed at 15% ambient oxygen level. Simultaneous planar laser-induced fluorescence (PLIF) of formaldehyde and schlieren imaging techniques were employed to analyze the ignition and flame characteristics experimentally. These studies revealed almost similar heat release rates for a double injection at 900 K and 800 K ambient gas temperatures due to combustion of a longer main injection which is enhanced by pilot combustion event. A lower soot production for 800 K ambient condition over 900 K case was observed, which was concluded to be due to its higher lift-off length which would allow for a leaner combustion of fuel-air mixtures. Numerical simulations were performed using a Large Eddy Simulation (LES) approach by extensively validating the 900 K double injection condition with respect to non-reacting vapor penetration profiles of both injections, reacting jet heat release rate and spatial as well as temporal (qualitative) soot production. As part of LES work, a dwell time variation of 0.65 ms (0.3/0.65/1.2 ms) was performed to reveal the sensitivity of soot production to variations in dwell time. It was observed numerically that marginally higher quasi-steady lift-off length of the 0.3/0.65/1.2 ms injection causes increased entrainment of surrounding oxygen into the flame region. This leads to combustion of slightly leaner fuel-air mixture and hence relatively less soot when compared to a 0.3/0.5/1.2 ms injection.

Keywords: Double injection; Soot; Ignition; Lift-off; Diesel spray.

1. Introduction

Modern compression ignition (CI) engines have been increasingly using new technologies to work around the problems of balancing low emissions, higher power output, and lower engine noise. Multiple injection technology has been a practically feasible way to mitigate these issues in both conventional diesel and gasoline type of Internal Combustion (IC) engines [1-3]. Interactions between the individual injections in a close-couple multiple injection event are a key to the resultant beneficial effects of emissions reduction, heat release phasing for high power output, and reduced engine noise.

Studies with multiple injections carried out in the past put forward interesting findings. It was found that in the case of a short dwell time, interaction of the velocity fields of the individual injections leads to an increase of the mixing rate at the second injection front [4]. Studies of non-reacting multiple injections revealed that the second injection liquid-phase penetration is longer than that of the first injection of the same duration [5], and also the vapor phase velocity of the second injection is higher than the first injection [6]. These phenomena are explained by the faster propagation of the main stream in an ambient provided by the vaporized pilot stream without the formation of a stagnation plane. For a reacting spray case, the ignition delay of the second injection is reported to be shorter than the first injection [6-8]. This reduction of the ignition delay was reported to be caused by the entrainment of high temperature gases from the combustion of the first injection into the main injection stream [4, 6].

It is also quite logical for the main injection to have a lower ignition delay since after the pilot ignition, the pressure and local temperature in the chamber increases, creating favorable conditions for the main injection to ignite sooner [9]. In such a scenario, even if the first injection is essentially soot-free, polycyclic aromatic hydrocarbons (PAH) and soot can be formed in the second injection due to the fuel rich combustion of the main injection. Reduced carbon-monoxide (CO), unburned hydrocarbons (UHC) and NO_x emissions were also reported [1, 2] due to implementation of multiple injections. This is largely due to a combined effect of the reduced ignition delay and fuel-air mixing of the subsequent injection. At the same time, specifically in the case of a double injection, due to the inhibited mixing of fuel and air, as the main injection enters the pilot zone,

increased PM (soot) emissions due to rich ignition of the main spray were also observed for some double injection cases [10]. But this deficiency can be tackled by the addition of a “post” injection after the main injection event to eventually reduce PM emissions [3]. By investigating the soot formation processes in a double injection, it would be convenient to understand the controlling processes in a triple or any other multiple injection scheme.

The present study is a follow-up of a series of studies as in Refs. [7, 11] in which extensive experimental and computational fluid dynamics (CFD) studies were performed to understand the ignition and sooting characteristics of multiple injections. As part of the experimental campaign, a single-shot PLIF imaging technique is used along with simultaneous application of high-speed schlieren imaging technique within a single injection cycle, to reveal the ignition and soot production characteristics of the main injection. PLIF is single-shot technique capturing image at the desired time instance while schlieren is a high-speed imaging technique capturing series of images of the entire combustion event. A Large Eddy Simulation (LES) based turbulence modelling approach was employed to provide unique insights into the double injection combustion process as explained later in section 3.2. The LES calculations have been extensively validated against single injection dataset for various ambient gas temperatures in prior works [12, 13]. Validations of the LES approach have been done in this paper for double injection scenario. The work is then extended to simulate dwell time variations of multiple injections in later part of this study in an attempt to understand the mechanism behind the change in soot production with dwell time variations.

The paper presents the experimental and numerical setups to begin with, followed by experimental results at 900 K and 800 K ambient cases. This is followed by CFD validation section of 900 K ambient case using LES model, after which a dwell time variation case of 0.65 ms is investigated for reduced net soot production.

2. Experimental and Numerical Approaches

2.1 Experimental setup

A constant combustion vessel (CV) with optical diagnostics was employed to investigate the double injection spray combustion event of n-dodecane (diesel surrogate). A high-pressure and high-temperature ambient environment, replicating the thermodynamic condition of a diesel engine, is obtained by burning a pre-calculated composition of premixed hydrocarbon mixture. A detailed description of the combustion vessel can be found in Ref. [14].

In the present work, the ambient of 15% oxygen in the chamber after the burning of premixed hydrocarbon mixture signifies the usage of exhaust gas re-circulation (EGR) in a diesel engine. EGR usage causes a net molar reduction of oxygen level (from a natural ambient of 21% oxygen) in the combustion vessel. The other ambient conditions of 22.8 kg/m³ ambient density and 800 K, 900 K of ambient temperatures are typical ambient conditions of a light-duty diesel engine at the time of fuel injection.

As part of experimental optical diagnostics, simultaneous acquisition of schlieren and PLIF imaging was performed as shown in Fig. 1

A Photron Fastcam SA1.1 high-speed camera operating at 37500 fps with a 26.67 μ s exposure time captures schlieren and luminosity images. During schlieren experiments, an LED (white 5500-K color temperature type) provides broadband collimated back-illumination by passing the source through a converging lens and a pin-hole aperture before it is reflected from a 750-mm focal length, 152-mm diameter parabolic mirror. The collimated beam then passes through a 50/50 beam splitter before entering the vessel through the combustion vessel sapphire window. The 50/50 beam splitter is used to reflect the fluorescence signal onto an intensified CCD (ICCD) camera, which will be described in more detail later. After passing through the spray chamber, the schlieren light is reflected by a flat mirror towards a second parabolic mirror. The converging/diverging beam then passes through a partial schlieren stop, placed at the focal length of the parabolic mirror, before entering a negative bi-convex lens (F.L. 200 mm) and then the 85-mm f/2.8 Nikkor camera lens. The negative bi-convex lens acts as a focusing lens. An optimal schlieren stop of 10-mm diameter was determined by trial and error. The high speed camera is equipped with a 600-nm short pass filter to capture only the highest intensity flame and (hotter)

soot emission. The image acquired had a projected pixel size of 0.156 mm/pixel. This constitutes the setup for the modified Z-type schlieren setup.

Fluorescence from formaldehyde (CH_2O) and polycyclic aromatic hydrocarbons (PAH) along the central plane of the spray axis is induced by a 54-mm wide, 0.4-mm thick sheet of 10-Hz (10-ns pulse) 355-nm laser light. The 355-nm pulses are generated from the third harmonic of an Nd:YAG laser with an average pulse energy of 95 mJ or a fluence of 0.44 J/cm^2 . Previous work has shown that this energy fluence is sufficient to achieve saturation of the formaldehyde fluorescence [15]. A gradually diverging (in width) laser sheet is formed by a set of spherical and cylindrical lenses. Before the laser sheet becomes too wide, the laser is reflected through the bottom vessel window by a 355-nm mirror. Fluorescence emitted from the spray flame is reflected by the aforementioned 50/50 beam-splitter onto an ICCD camera. The ICCD camera is equipped with a 400-nm (20 nm FWHM) bandpass interference filter to capture the fluorescence signal from the formaldehyde and PAH species. It is a single shot ICCD camera with an exposure time set at 100-ns.

One of the advantages of the PLIF technique for formaldehyde detection consists of the fact that it can also detect PAH formation, since signal detection wavelengths for both species are close to one another [16, 17]. Usually, PAH is formed at a different spatial location than formaldehyde which makes the PLIF technique useful to detect the formaldehyde presence and to differentiate it from the PAH signal [18]. Also, PAH appears in a 'saturated' fashion. This is because, the formaldehyde signal is a lower magnitude signal and stops rising in intensity at a certain threshold, unlike PAH/soot signal, which can rise until higher magnitudes thus appearing saturated in a formaldehyde PLIF image. More details including the implementation of PAH and formaldehyde PLIF are discussed in Sec. 3.1.

The pressure trace from the CV was also recorded. A single-hole solenoid injector (Injector# 375020) from the Engine Combustion Network (ECN) [19] community was used to create multiple injections using a MOSFET driver. The rate of injection (ROI) was experimentally determined using spray momentum flux measurements [20]. In the ROI measurements, injection is done onto the face of a force transducer. Using momentum relationships, the mass flow rate of injection is back calculated. As can be seen in Fig. 2, the rate of injection profile, shows a

0.3 ms injection of pilot spray, a 0.5 ms of dwell time and a 1.2 ms injection of main spray, giving it the nomenclature of 0.3/0.5/1.2 ms. The measured ROI profile has noise arising from experimental artifacts. To avoid this noise to bleed into the CFD simulations, a standardized rate of injection (ROI) profile from CMT-Motores Térmicos [21] was used as the CFD input, as seen in Fig. 2.

2.2 Numerical approach

In this work, LES was performed through a Lagrangian-parcel, Eulerian-fluid approach using the CFD software CONVERGE [22]. The LES governing equations are discretized spatially using a second order finite volume scheme and temporally using the PISO (Pressure Implicit with Splitting of Operators) scheme. A base grid size of 1 mm is used along with local embedding of 62.5 μm in the form of a cylinder with diameter of 4 mm and height of 5 mm near the nozzle. Adaptive mesh refinement (AMR) is also used and gets activated whenever the sub-grid velocity gradient is higher than 0.1 m/s or the sub-grid temperature gradient exceeds 2.5 K. This setup leads to a 62.5 μm grid in the entire spray and flame region with grid-convergent results [13]. The dispersed phase is modeled using the traditional Lagrangian-parcel method. More details about the spray models employed in this study are discussed in detail in Refs. [12, 13] and hence the governing equations are not discussed here for the sake of brevity.

A well-mixed turbulent combustion model is employed. The chemical kinetics are modeled using a 54-species, 269-reaction mechanisms for n-dodecane [23]. The present work uses a Hiroyasu model [24] to simulate soot formation and Nagel Strickland-Constable (NSC) model [25] to simulate soot oxidation. Acetylene (C_2H_2) is chosen as the soot precursor which makes soot formation rate linked to the mass fraction of C_2H_2 . The net soot formation is a competition between soot formation and soot oxidation. The Hiroyasu model is a single step model given by Eq. 2 as

$$\dot{M}_{sf} = A_{sf} P^{0.5} \exp\left(-\frac{E_{sf}}{R_u T}\right) M_{form} \quad (1)$$

Where $\dot{M}_{sf}$ is the soot formation rate in g/sec, M_{form} is the mass of soot formation species (C_2H_2) in grams, P is the cell pressure in bar, R_u is the universal gas constant in cal/(kg-mol), T is the cell temperature in K, E_{sf} is the

activation energy in cal/g-mol, and A_{sf} is the Arrhenius pre-exponential factor with units of $1/(s\text{-bar}^{0.5})$. Thus, as soon as C_2H_2 starts forming, there will be some presence of soot detected in the computational cell.

The NSC soot oxidation model is a single step model given by Eq. 3 as

$$\dot{M}_{so} = A_{so} \frac{6M_s}{\rho_s D_s} R_{total} MW_c \quad (2)$$

$\dot{M}_{so}$ is the rate of oxidation of soot species, MW_c (g/mol) is the molecular weight of carbon, A_{so} is a scaling factor, M_s is the total soot particle mass in grams, ρ_s is the soot density in g/cm^3 , D_s is the nominal soot particle diameter and R_{total} is the net reaction rate, which is a function of partial pressure of O_2 and temperature.

The effect of the sub-grid fluctuations are incorporated using the well-validated one-equation dynamic structure sub-grid scale (SGS) model [26]. This computational setup has been employed in previous studies Refs. [12, 13] for LES of a single injection of n-dodecane and it was shown that the model is able to predict ignition delay, lift-off length and soot contours accurately. A total cell count of 22 million was observed at 2 ms after start of injection (ASOI) time for the 0.3/0.5/1.2 ms case. Until 2 ms ASOI, the 0.3/0.5/1.2 ms case consumed ~48,000 core hours with ~20 days of wall-clock time. It is to be noted that, LES results in this study are based on a single realization and accurate *quantitative results* can only be obtained by performing multiple realizations. However, a single LES realization can provide valuable *qualitative description* of the flame development as noted in author's previous studies [12, 13, 27].

3. Results and Discussion

Table 1 shows the ignition delays from the experimental cases of 900 K and 800 K ambient gas temperatures and the 900 K CFD case for two dwell time variations.

The 900 K CFD case was extensively validated against the experiments which will be discussed later. The ignition delay of the first injection is calculated from the pressure trace corresponding to the first increase of pressure by 0.024 bar. However for the second injection, ignition delay was calculated after the start of main injection (ASMI) where the apparent heat release rate increases by 20% from the value at the minimum near the main

injection timing following Skeen et al. [6] recommendation. More than two-fold increase in ignition delay is observed for the pilot injection going from 900 K to 800 K ambient. The ignition delay for the second injection is almost half of the pilot injection for the cases shown in Table 1.

3.1. Simultaneous schlieren and PLIF imaging

Fig. 3 shows the raw simultaneous imaging of PLIF and schlieren acquired in a nearly simultaneous fashion. The HS schlieren with natural luminosity image is acquired with a 600 nm short pass filter on the high-speed camera. The 600 nm short pass filter enabled the visualization of only the high temperature soot species along with other minor species which emit in the wavelengths lower than 600 nm.

The images comprising formaldehyde PLIF in Fig. 3 are not from the same injection event since the ICCD camera can only capture a single shot. Separate injection and pre-burn event were needed to obtain each ICCD image to realize 3 repeats for the same test condition. The mean image of the 3 repeats is used for presenting results here. While one ICCD image was being taken, a high-speed (HS) schlieren movie was recorded for the whole injection-spray-combustion event. The HS schlieren image shown on the right has been extracted from one of the three repeats for the corresponding ICCD PLIF shot. These are called simultaneous since at least one (out of the 3 repeats) ICCD image lies in the same injection cycle to one schlieren image. The liquid length section is shown covered by a shaded region in Fig. 3. From run to run, the overall flame structure characteristics (flame length, intensity magnitude, flame width, etc.) are not significantly varied and are fairly repeatable while there are some variations in the internal structure as expected. The penetration of the downstream hot flame and upstream cool flame, and the overall shape of the PAH in jet head and CH_2O in the upstream near region looks very similar between the 3 repeats. This was seen in other test results too. Hence, only 3 repeats were performed in the experiment to maintain minimum statistics. Slight liquid scatter is observed in the PLIF shots near the nozzle during the liquid injection durations as can be seen within the masked zone, signifying liquid length extent in the PLIF images of Fig. 3. Although this very weak fluorescence signal was observed near the nozzle from liquid fluorescence, the downstream target measurement (after the masked zone) is not mixed with

this signal, as seen in the Fig. 3 and so is unambiguous in deciding that downstream signal was a formaldehyde (PAH) signal and not a fuel liquid scatter.

Fig. 4 shows the schlieren-PLIF imaging for 900 K ambient case using 0.3/0.5/1.2 ms injection strategy. A dashed line in the top-right PLIF image sets indicate the quasi-steady lift-off. Points of interest have been marked in Fig. 4 with circles. Point 1 corresponds to schlieren softening (right image set), which indicates large-scale organization of vaporized fuel mass, possibly with similar equivalence ratios and fluid temperatures, ready to undergo a first stage ignition.

This first stage ignition is visualized as a formaldehyde signal (left image set). Point 2 shows luminosity occurrence in the right image set which constitutes of soot matter as well as its precursor species (PAH) as seen from the left image set. This is one of the advantages of the PLIF technique for formaldehyde detection since the signal detection wavelength of PAH lies close to that of formaldehyde [28], which enables visualization of both these species simultaneously. Usually, PAH is formed at a different spatial location than formaldehyde, which makes the PLIF technique useful to detect the formaldehyde presence and to differentiate it from the PAH signal, as in this case. From the time instants of ~ 0.79 ms and ~ 0.9 ms (from both HS and ICCD images), one can visualize the ambient conditions in which the main injection enters the combustion vessel, as further explained here. A combustion recession event [29] of the pilot is happening with no evidence of reactive radicals (signified by formaldehyde presence) in the immediate ambient of the main injection. Combustion recession is an end of injection transient phenomena where shortly after the end of injection, under high-temperature ambient combustion conditions, the recently prevalent lifted flame seemingly propagates back towards the injector. This is due to the generation of auto-ignition spots upstream at end of injection times. Thus, combustion recessing is a series of high temperature ignition events, which occur upstream thus consuming the low-medium temperature reactive species (signified by formaldehyde). The presence of local high temperature due to combustion recession existing near the main liquid fuel injection leads to earlier ignition in a fuel-rich manner, leading to more PAH and soot formation downstream. Point 3 signifies the after end of injection times where combustion recession [29] starts to occur for the main injection. As this happens, the left over upstream low and

medium temperature main reactive species (with low axial velocities) experience an immediate increase in their production and are soon exhausted as temperature rises with high temperature chemical reactions occurring. Thus, a higher level of formaldehyde trace is seen upstream in the region marked as point 3 (left image set) which gets consumed in later time instants.

Fig. 5 shows simultaneous schlieren-PLIF imaging at 800 K ambient. Point 1 here shows the development of first-stage ignition kernels in the form of a cool flame signified by formaldehyde presence from the formaldehyde PLIF. These first stage ignition kernels travel downstream and later auto-ignite (as point 2) producing high temperature combustion species (CO, OH etc.).

From the time instants of ~ 0.78 ms and ~ 0.97 ms (both from HS and ICCD), one can visualize the ambient in which the main injection enters the combustion vessel. A spatial presence of low temperature reactive radicals (signified by formaldehyde presence) lies in the immediate vicinity of the main injection, unlike the high temperature ambient for the main injection for the 900 K ambient case (cf. Fig. 3). Skeen et al. [6] performed closed homogenous reactor simulations which took inputs such as local equivalence ratios from a one-dimensional jet model to investigate the effect of high-temperature and reactive radicals on main ignition. They concluded that both the temperature and reactive radicals can have effects on reducing the main ignition delays in almost similar magnitudes. Thus the reduction in ignition delays of main by almost a factor of two over pilot are imminent (cf. Table 1). This promotes the PAH and soot formation due to the nature of fuel rich ignition. The dashed line in the top-right PLIF image set in Fig. 5 shows the lift-off location. It can be observed that the quasi-steady lift-off location in the 800 K ambient case is further away from the nozzle (21 mm) when compared to the 900 K case (13 mm).

From Table 1, it is observed that the ignition delays for the 900 K case for both injections are lower than the 800 K case. The associated quasi-steady lift-off length behavior with the ignition delay trend as seen in both the cases, here is expected from previous well established studies [30] that were primarily for single injection sprays, but can be extended to double injection sprays. It was also found for a single injection diesel spray that the total amount of air entrained upstream of the lift-off length increases due to an increase in lift-off length

with decreasing ambient gas temperatures [31]. Using empirical laws derived from multiple datasets, Siebers [31] concluded that higher lift-off lengths cause higher air entrainment, which leads to a leaner central reaction zone at near-downstream locations of the lift-off length. Leaner conditions cause less soot formation (as seen in the 800 K case of Fig. 6). This theory will be put to use in the upcoming CFD discussion section.

Temporal and spatial flame luminosity was calculated by integrating flame luminosity at each axial location for each frame of a natural luminosity acquired image as in Fig. 6. This is named as an IXT (Intensity-aXial-Time) plot defined mathematically as in Eq. 1.

$$IXT(x, t) = \int_{-R}^R I(x, r, t) dr \quad (3)$$

where x is the intensity axial direction, r is the radial direction, and R is intensity boundary width. Aspects such as lift-off length, flame height, and some aspects of internal flame structure can be studied by the IXT contours. IXT plot has been employed in the previous study by the authors [7] to explore the flame luminosity profile of various multiple injection sequences. Also plotted in Fig. 6 are the apparent heat release rate (AHRR) profiles for the same cases.

The CV pressure trace is used to determine the AHRR from the combustion event. The AHRR profiles are a mean of 3 tests for each condition. The relationship used in the AHRR calculated is provided by Eq. 4.

$$\frac{dQ}{dt} = \frac{\gamma}{\gamma-1} P \frac{dV}{dt} + \frac{1}{\gamma-1} V \frac{dP}{dt} = \frac{1}{\gamma-1} V \frac{dP}{dt} \quad (4)$$

where P is chamber pressure, V is the combustion vessel volume (1.1L), and γ is specific heat ratio (1.35). The combustion efficiencies calculated for both the 900 K and 800 K injection cases come close to 92% although major qualitative differences in the soot production are observed in Fig. 6, where the 900 K case (shown in gray scale) has a higher level of soot production than the 800 K case (shown in RGB scale). Additionally, in the 800 K case, the pilot does not exhibit any soot luminosity, and becomes evident only during the end of main spray

injection times. Also, the fact that the main injection stabilizes at a lesser lift-off length than the pilot injection is observed in Fig. 6 for the 900 K case.

3.2. Simulation of 900 K case with varying dwell times and validation

The effect of changing the dwell time was investigated using a well validated CFD simulation against the 900 K case of a 0.3/0.5/1.2 ms injection. The validation process consisted of considering both the non-reacting and reacting spray parameters which include vapor penetration (of both the injections), heat release and qualitative soot presence. Simulations for the reacting cases were performed until end of injection times.

Fig. 7 shows the non-reacting vapor penetration which was performed to validate the vaporizing spray before setting up a reacting case. LES calculations can predict the vapor penetration very well for both the injections. This is consistent with authors' previous findings for single injection simulations with LES [27]. It can be noted from experiments that the main injection travels faster than the pilot injection, since the slope of the second injection is higher than the first injection. This was termed as 'slip stream' effect [6], since the main injection is now traveling in a spray cooled field of higher density created by the pilot injection and hence slips through it quicker than it would in a lower density hot gas. The simulation captures this phenomenon very well. At the bottom of Fig. 7, the AHRR profiles are shown. The CFD heat release plotted here is not the chemical heat release but the pressure-derived (apparent) heat release, as done in the experiments. The plots show overall good agreement between simulations and experiments.

Fig. 8 shows a comparison of line-of-sight integrated IXT plot for natural luminosity imaging with a similarly plotted soot plot from CFD.

For the CFD soot mass spread, the soot mass along the line-of-sight has been integrated and projected on a plane. This which was considered for transverse integration operations along the axial length for the various time steps leading to the plot in Fig. 8 (right). Luminosity visualization with a 600 nm short pass filter does not directly correlate to soot particle measurements as in a laser incandescence measurement, but is a good indication of high temperature or high concentration soot. Fig. 8 depicts that it is a good estimate for qualitative

indication of soot presence. The start of soot production (along X-axis) and the flame lengths containing soot (along Y-axis) are very well matched between CFD and experiment.

Simulation of a double injection spray-combustion event has been a challenge within the spray-flame community and was an issue of interest in the ECN 4 workshop as well [32]. In view of this, involving high fidelity LES calculations with a detailed chemistry well-mixed combustion model is believed to be a good approach.

Using this well validated CFD simulation, a variation in dwell time was performed. The dwell time was increased from 0.5 ms to 0.65 ms at 900 K ambient gas temperature, with the injection durations being the same. The ignition delay of the main injection in this case was 0.165 ms which is 0.025 ms longer than the 0.3/0.5/1.2 ms main injection (ignition delay: 0.14 ms). The lift-off lengths for the main injection for both dwell time variations were calculated from the 14% OH magnitude, at the farthest upstream position of its presence [33] to account for similarity with experiments. These were calculated as 22.4 mm for the 0.3/0.5/1.2 ms case and 24.6 mm for the 0.3/0.65/1.2 ms case for their respective main injections. Although the simulation shows higher lift-off length, the simulation set-up correctly predicts the change in lift-off lengths with changing ambient conditions [13]. Hence, the conclusions derived from LES are expected to hold good in spite of the differences in predicted lift-off lengths.

Fig. 9 shows the heat release rate of the various 900 K cases investigated. It can be observed that as the dwell time is increased (by 0.15 ms) in the simulations, there is a delay in the start of heat release from the second injection. The difference in the behavior of heat release rate begins at 0.8 ms ASOI, until when both the dwell time cases have identical heat release. It is seen that the pilot injection still has the potential of releasing heat after 0.8 ms which was rather quenched by the oncoming main injection for the 0.3/0.5/1.2 ms case. Thus, as the dwell time is increased by 0.15 ms, the heat release rate during the dwell time is seen to be marginally higher for the 0.3/0.65/1.2 ms case. At the same time the 0.3/0.65/1.2 ms case takes longer to achieve the eventual rise in heat release rate from the second injection which now occurs at ~ 1.1 ms ASOI, in contrast to ~ 0.9 ms ASOI for the 0.3/0.5/1.2 ms case. This change in behavior of heat release rate from the second injection

due to the variation in dwell time, effects the spray-flame in general, and main soot formation characteristics in particular.

The upcoming analysis deals with investigating how changes in the dwell-time affects the soot formation on a *qualitative* sense. Multiple LES realizations are needed for *quantitative* comparisons with experiments. In previous work done by Pei. et al. [13], it was found that that ignition delay is fairly repeatable from realization to realization, whereas there can be up to 5 mm variation in lift-off length from one realization to the next for a single injection case at similar experimental conditions with n-dodecane as fuel. However, this study is geared more towards getting a qualitative sense of soot dependence when the dwell time is changed. Hence, at many places qualitative terms like 'percentage change' are used rather than absolute measurable quantities.

Fig. 10 (top) shows a schematic for calculation of air entrainment rate. A cell flowrate-weighted radial mean value of the equivalence ratio enclosed in a region bounded by 0.1% mixture fraction surface was obtained at the lift-off location. An inverse of such equivalence ratio was estimated as an air entrainment quantity, following Siebers and Higgins [31]. Azimov and Kim [34] have performed air-entrainment estimate following a different approach involving direct mass measurements of air and fuel entrainments from their LES calculations. They had very close air-entrainment estimates as Siebers and Higgins [31], which is used in the present study.

For the quasi-steady main flame lift-off times for 0.3/0.5/1.2 ms case, an air-entrainment of 72.6% was obtained whereas the 0.3/0.65/1.2 case yielded 81.9% air-entrainment rate. The 12.8% increase in the air-entrainment of 0.3/0.65/1.2 ms case over 0.3/0.5/1.2 ms case is due to the lift-off length of the former main flame being 2.2 mm longer than that of the latter. The increased air entrainment may also arise from a higher radial expansion of the wider main flame observed for 0.3/0.65/1.2 ms case (not shown here), which creates a stronger entrainment current near the lift-off base location. This is one of the theories supporting an air-entrainment concept by Rhim and Farrell [35], who suggested that a significant part of the overall ambient gas is entrained from the downstream spray region. Thus, with more air entrainment, fuel leaning of the fuel-air mixture for the 0.3/0.65/1.2 ms case causes lower soot production as shown in Fig. 10 (bottom) where the solid lines show the soot mass. At end of the respective main injection times for the both the dwell time cases, the net soot

production was calculated to be ~14.2% lesser for 0.3/0.65/1.2 ms case over 0.3/0.5/1.2 ms case. A similar trend of reduction in soot production rates with increasing dwell times was observed by Hasse with a turbulence-chemistry interaction combustion model [9]. Thus, it can be said that a higher level of air entrainment causes slightly leaner combustion of the main spray for the 0.3/0.65/1.2 ms injection case than the 0.3/0.5/1.2 ms injection case, resulting in lesser soot production. The mechanism for air-entrainment for a multiple injection flame is expected to be a symbiotic relationship between the interaction levels of both the injections and the corresponding lift-off lengths for the varying dwell time cases.

4. Conclusions

Analysis of soot production trends for double injections of n-dodecane fuel in a controlled environment of constant volume combustion vessel was performed. Experiments done with 0.3/0.5/1.2 ms multiple injection scheme show the benefit of using a multiple injection to get higher combustion efficiency, while keeping soot in low-limits when the ambient gas temperature is reduced from 900 K to 800 K. Integrated intensity plots provided a convenient way to gauge the qualitative soot trends in the cases tested. A reduction in ignition delay of the main injection by almost a factor of two over pilot was observed for both the 900 K and 800 K ambient conditions. Ignition and stabilization of the main spray-flame closer to the liquid injection (fuel rich zone) was observed which results in its higher PAH and soot formation downstream. For 900 K condition, the reduction in main ignition delay is believed due to the high temperature combustion recession event in which the main injection is injected. For the 800 K case, the reduced ignition delay is believed to be due to the local presence of pilot generated low temperature reactive species signified by the formaldehyde presence. Simulation of a 900 K ambient gas temperature 0.3/0.5/1.2 ms injection was performed using a LES framework and extensively validated to simulate important multiple injection related mechanisms of slip-stream effect in non-reacting environments along with reduced main ignition delays, lift-off lengths and the general soot spread in reacting ambients. A slight increase in dwell time from 0.5 ms to 0.65 ms revealed a 14.2% decrease in soot production. A 12.8% increase in air-entrainment for the 0.3/0.65/1.2 ms case was found to predominantly cause lower soot

production. The increased air entrainment is due to an increased lift-off length along with stronger entrainment current generated near the lift-off base location from a higher radial expansion of the 0.3/0.65/1.2 ms main flame.

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Table 1: Ignition delay measurements from experiments and CFD

Experiment	Pilot ignition delay	Main ignition delay
900K: (0.3/0.5/1.2 ms)	0.27 ± 0.01 ms	0.16 ± 0.02 ms
800K: (0.3/0.5/1.2 ms)	0.58 ± 0.06 ms	0.21 ± 0.04 ms
CFD	Pilot ignition delay	Main ignition delay
900K: (0.3/0.5/1.2 ms)	0.26 ms	0.14 ms
900K: (0.3/0.65/1.2 ms)	0.26 ms	0.165 ms

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