

Combustion Recession after End of Injection in Diesel Sprays

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ABSTRACT

This work contributes to the understanding of physical mechanisms that control flashback, or more appropriately combustion recession, in diesel sprays. A large dataset, comprising many fuels, injection pressures, ambient temperatures, ambient oxygen concentrations, ambient densities, and nozzle diameters is used to explore experimental trends for the behavior of combustion recession. Then, a reduced-order model, capable of modeling non-reacting and reacting conditions, is used to help interpret the experimental trends. Finally, the reduced-order model is used to predict how a controlled ramp-down rate-of-injection can enhance the likelihood of combustion recession for conditions that would not normally exhibit combustion recession.

In general, fuel, ambient conditions, and the end-of-injection transient determine the success or failure of combustion recession. The likelihood of combustion recession increases for higher ambient temperatures and oxygen concentrations, as well as for higher reactivity fuels. The likelihood of combustion recession was further linked to the characteristics of end-of-injection entrainment. A simple equation, linking equivalence ratio at the lift-off length, $\phi(\text{LOL})$, with a dimensionless parameter related to the end-of-injection entrainment wave, was found to well predict the propensity for combustion recession of dodecane sprays over a wide range of experimental data and 1-D model predictions. Our results suggest that this relationship is $\phi(\text{LOL}) \sim D_{\text{eff}}/(\alpha U_{\text{eff}})^{0.474}$, where D_{eff} is the effective orifice diameter, α is the end-of-injection ramp-down duration, and U_{eff} is the effective injection velocity.

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INTRODUCTION

Unburned hydrocarbon (UHC) emissions under low-temperature combustion (LTC) operating conditions have recently been linked to the end-of-injection transient in diesel injectors and the impact of this transient on the combustion of near-nozzle mixtures [1, 2]. Specifically, it has been observed that air-fuel mixtures close to the injector nozzle may undergo first-stage or cool flame ignition, but do not eclipse to second-stage or high-temperature ignition, leaving a mixture of partially oxidized hydrocarbons that contribute to UHC [2]. This phenomenon has been strongly linked to positive ignition dwell LTC conditions, where the fuel injection event ends before combustion begins. Under such conditions, the lack of high-temperature ignition within the near-nozzle mixtures has been suggested to be the consequence of locally enhanced entrainment following the end-of-injection transient, which progresses downstream from the injector nozzle in the manner of an "entrainment wave" [1]. The entrainment wave rapidly leans mixtures near the nozzle such that these regions become incapable of supporting second-stage ignition.

The tendency for near-nozzle mixtures to resist a transition to second-stage ignition has also been observed for negative ignition dwell LTC conditions, where combustion begins before the end of injection [1]. Under these conditions, as shown schematically in the upper half of Figure 1, a lifted flame is observed to occur at a quasi-steady location downstream of the nozzle throughout the injection event, termed the lift-off length (LOL). Because LTC conditions are typically highly dilute, with ambient oxygen concentrations near 12-15%, increased mixing times are required to reach ignitable fuel-ambient mixtures. As a result, the lifted flame, or high-temperature reaction zone, occurs relatively far downstream of the nozzle [3]. After the end of injection, the position of the lifted flame can remain far downstream, leaving a large region of unburned or partially burned fuel-air mixture upstream [1]. Since the mass of fuel in the jet increases as the square of the distance from the injector under steady injection, the potential for UHC emitted increases as the square of the lift-off length. Thus, since lift-off lengths are relatively long for low-temperature combustion operating conditions, the lack of flame retreat after end-of-injection is a major concern.

Under high-temperature conventional diesel combustion operating conditions, however, there is evidence to suggest that the lifted flame does propagate back towards the injector after the end of injection [4, 5, 6]. As shown schematically in the bottom half of Figure 1, under high temperature low dilution ambient conditions, second-stage ignition reactions are observed in near nozzle mixtures despite locally enhanced entrainment accompanying the end-of-injection entrainment wave (indicated by larger entrainment arrows in the schematic). Multiple participants of the Engine Combustion Network (ECN) have observed this process, including Sandia National Laboratories and Eindhoven University of Technology, though no published works have focused on it [7]. Often, the phenomena is observed as shown in Figure 1, as a recession of the high-temperature reaction zone from the lifted flame position back towards the injector nozzle. This has lead researchers who have observed such phenomena to refer to this as “flashback” [1, 5]. This term has likely been used due to its commonality with similar lifted-flame phenomenon observed in gas-turbine studies. However, as we will show in this work, under typical diesel engine operating conditions, autoignition rather than flame propagation may play a dominating role. Thus, combustion recession is adopted as a more general term to describe this phenomenon [4].

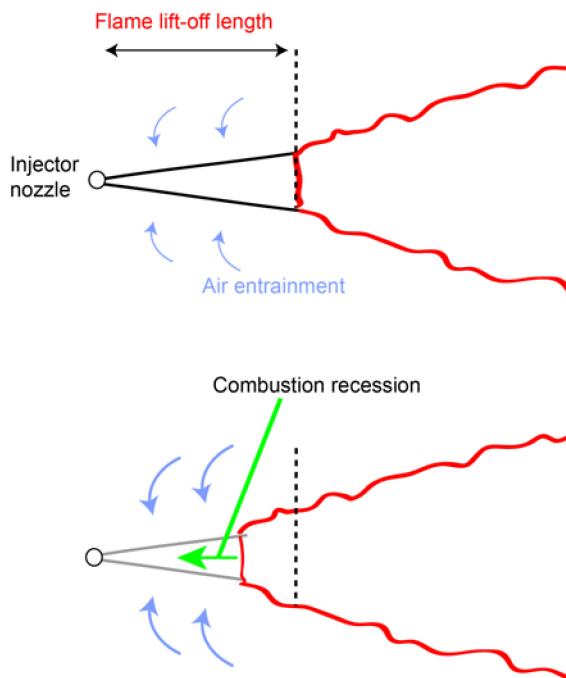


Figure 1. Schematic of combustion recession

As previously discussed, the advent of low-temperature combustion and the associated effects of end-of-injection over-leaning and UHC emissions have been primarily responsible for motivating an interest in end-of-injection combustion recession. In fact, combustion recession can be observed in the early optical engine studies of Espey and Dec [8], but it has been given little attention to date. This is likely due to the fact that their experiments were under conventional, or high-temperature, combustion conditions which are more likely to exhibit combustion recession. Moreover, even if combustion recession were not observed, the potential for UHC is low because high-temperature combustion lift-off lengths are short. Now though,

optical engine studies are aimed directly at examining the fate of upstream near-nozzle mixtures and their impact on UHC [1, 2]. These findings suggest a dominating trend towards lack of combustion recession under low-temperature combustion conditions, warranting an interest in understanding the nature of these end-of-injection combustion transients and the conditions which support or suppress combustion recession.

Though there have been no known targeted studies on the conditions that either support or suppress combustion recession, prior research on end-of-injection soot behavior provides further evidence for a transition to no combustion recession for highly dilute or LTC conditions. Bobba, Genzale, and Musculus measured the spatial and temporal development of soot luminosity and observed that as the top-dead-center motored temperature decreased from 1000 K to 875 K, transitioning from high to low-temperature combustion conditions, the soot luminosity stopped retreating back toward the injector after end-of-injection [5]. While not specifically addressed, soot imaging by Singh, Reitz, and Musculus also show a similar change in the behavior of soot recession between high and low-temperature combustion operating regimes [6]. While the observation of soot recession from these natural luminosity measurements is an indicator that combustion recession has also occurred, chemiluminescence from ignition radicals is much weaker than soot luminosity and would not likely be captured by these measurements. Thus, the ambient conditions where a transition from combustion recession to no combustion recession occurs cannot be readily identified from these measurements. High-sensitivity chemiluminescence imaging, like that used in [1], or an indirect measurement of mixture temperatures from schlieren [9], is needed to resolve the relatively weak emission from combustion radicals without interference from soot.

Other work focused on the impact of end-of-injection transients on near-nozzle fuel-ambient mixing and liquid vaporization suggests that, in addition to ambient conditions, the characteristics of the end-of-injection mass flow rate will influence the likelihood of combustion recession. Kook, Pickett, and Musculus have demonstrated that the liquid penetration length also undergoes a recession back towards the injector from its quasi-steady value during the end of injection [10]. Using a 1-D mixing model, they showed that the details of the entrainment wave dictate the behavior of liquid length recession. Specifically, they show that the speed and magnitude of the entrainment wave affect local mixing rates, which determine the liquid penetration distance and the liquid recession rate. Further, they show that the speed and magnitude of the entrainment wave is controlled by the injection velocity, nozzle orifice area, and injector closing duration. Higher injection pressures and larger nozzle orifice diameters were both shown to decrease the liquid penetration distance and increase the liquid recession rate. However, the injector closing duration was demonstrated to increase the liquid penetration distance and decrease the liquid recession rate. Extrapolating from their results, it is expected that combustion recession behavior should also be controlled by the end-of-injection entrainment transient in the jet because ignition reactions are sensitive to the relative amounts of fuel and ambient gases.

The objective of this work is to identify ambient and injection conditions that support and/or suppress combustion recession in order to develop fundamental insight on the nature of combustion recession. Diagnostics are employed that are sensitive to reactive species, without interference of soot, including high-speed chemiluminescence and schlieren imaging during the end-of-injection transient. A large dataset is used, primarily centered on a sweep of ambient and injection conditions surrounding the ECN Spray A condition [7], to develop trends of the existence of combustion recession as well as the time required for combustion recession at each condition. Since the dataset can be sparse for certain conditions, identification of areas that need further attention is another major goal of this work.

EXPERIMENTS

Experiments were performed at two institutions, namely Sandia National Laboratories (Sandia) and CMT - Motores Térmicos (CMT). Below, we summarize the experimental facilities and diagnostics employed at each institution to measure combustion recession. The fuel injection and ambient operating conditions studied are also summarized.

Spray Combustion Vessels

Data was obtained in two optically-accessible combustion vessels; one is a pre-burn, constant-volume type vessel used at Sandia [11] and the other is a flow-through constant-pressure type vessel employed at CMT [12]. Both are capable of simulating the ambient conditions inside of a diesel engine at top-dead-center condition. Table 1 contains several columns of experimental conditions where the subscript of each denotes which facility the measurements were completed. A subscript of 1 denotes the pre-burn constant volume vessel at Sandia and a subscript of 2 denotes the flow-through constant pressure vessel at CMT. A detailed comparison of these vessels, including diagnostics used in this paper is given in Refs. [13] and [14].

Fuel Injectors

A common rail fuel injector, the so-called Spray A injector, was used for the majority of the experiments performed at Sandia and CMT. This injector is used within the ECN group, an international collaboration among different research laboratories around the world [11]. The injector has a single-orifice nozzle with a nominal diameter of 90 μm . The experiments performed at CMT were conducted with a specific injector, namely model #675. Additional single-orifice, mini-sac-type injector tips similar to Spray A were also used for experiments at Sandia. The orifice diameter for each injector tip is shown in Table 1. Detailed information about the nozzle shapes are available at [7].

The measured end of injection transient for Spray A is shown in Figure 2, where time is given relative to the start of ramp down in injection rate [7]. Throughout this work, time will be given after start of ramp down (aSOR) because after this instance changes in the mixing due to the end of injection will then have an effect of combustion. The ramp down process lasts approximately 100 μs and

is reasonably linear during this period. Note that time zero is positioned at the instance when the rate-of-injection drops below its steady-state value, reflecting the start of the end-of-injection transient. As shown in Figure 2, due to acoustic pressure oscillations in the fuel system, fluctuations in the steady-state injection rate are observed. Thus, the steady-state injection rate is quantified by taking an average of the measured rate-of-injection from -4000 (not shown) to $-100 \mu\text{s}$ aSOR. The positive values of the injection rate seen between 100 μs and 300 μs are most likely an artifact of the rate-of-injection measurement device. As shown and discussed later in Figure 4, there is no evidence of liquid fuel at these times in high-speed imaging measurements. Therefore, we have considered injection to completely end when the rate of injection signal crosses zero near 100 μs aSOR.

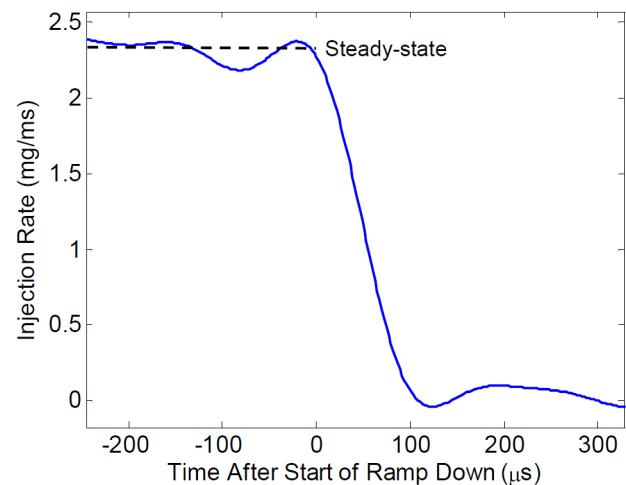


Figure 2. Measured rate of injection for Spray A [7]

Fuels

Several single-component, binary-blend, and multi-component fuels were used in this work. The binary blend was a gasoline-type primary reference fuel (PRF) consisting of n-heptane and iso-octane where the percentage of iso-octane is denoted, e.g. PRF20 [15]. The gasoline was locally available and details of the diesel fuel are available at [7].

Test Conditions

A large range of test conditions have been explored for the experimental data used in this study. The goal of such a large test matrix is to observe trends in the behavior of combustion recession as conditions are transitioned from low to high-temperature combustion operating conditions. As previously stated, the data is a combination from two sources, Sandia and CMT.

Two conditions of relevance to the diesel engine community that have been agreed upon by the ECN are termed Spray A and Spray H. Table 1 encompasses both conditions as well as parameter variations on each. The baseline Spray A condition is defined by the use of n-dodecane as fuel, a nominal 90 μm single, on-axis orifice with k-factor of 1.5, 150 MPa injection pressure, 22.8 kg/m³ ambient density, 900 K ambient temperature, and 15% ϕ equivalence ratio. The baseline Spray H condition includes the use of

n-heptane as fuel, a nominal 100 μm single, on-axis cylindrical orifice, 150 MPa injection pressure, 14.8 kg/m³ ambient density, 1000 K ambient temperature. More details on each condition can be found in [7].

Table 1. Test conditions for combustion recession data. Each column has a subscript to denote in which facility the measurements were completed. A subscript of 1 denotes the pre-burn constant volume type [11] and a subscript of 2 denotes the flow-through constant pressure type vessel [12].

	N-heptane _{1,2}	Diesel ₁	Gasoline ₁	Dodecane _{1,2}	PRF20 ₂
Nozzle diameter (μm)	100, 90	90, 110, 180	180	90	90
Ambient temperature (K)	850 - 1000	800 - 1200	900 - 1300	750 - 1200	800 - 950
Ambient density (kg/m ³)	14.8, 22.8	14.8, 22.8	14.8	7.6 - 22.8	22.8
Ambient O ₂ (%)	15 - 21	15 - 21	21	13 - 21	15 - 21
Injection pressure (MPa)	150	90 - 150	90	30 - 150	50 - 150

Diagnostics

Two optical techniques are used to detect and identify combustion recession. A key feature of these techniques is that they are high-speed so that the combustion recession process can be resolved in time.

A broadband chemiluminescence imaging setup was used to detect a large range of electronically-excited species that appear at the onset of high-temperature combustion [16, 17, 18]. To focus on the recession of ignition rather than soot, rejection of soot luminosity was achieved with a 600-nm short-pass filter using the setup provided in Bardi et al. [14]. This filter allowed for the collection of electronically-excited radicals, e.g. CH* and C2*, while eliminating a portion of the emission and background flare due to soot incandescence in the lift-off region. As detailed in Ref. [14], visible-wavelength emission can be reliably utilized to identify high-temperature ignition timing because soot luminosity occurs after autoignition. When overall soot luminosity is low and it occurs downstream of the lift-off length, chemiluminescence at the lift-off length may also be measured after ignition, as demonstrated in Ref. [19]. In addition, dynamic background corrections were implemented in this study to distinguish combustion chemiluminescence from the soot luminosity flare reflected outside of the spray, as detailed in [20].

Schlieren imaging was used to identify regions of high-temperature products near the injector after the end of injection that result from combustion recession. Schlieren is a line-of-sight technique that is sensitive to index of refractive gradients anywhere along the beam path. Unfortunately, thermal gradients at the windows of the combustion vessel are also visible, which creates a slowly evolving and noisy background. The Sandia schlieren setup is more sensitive to schlieren disturbances, with more details given in Ref [14].

Consequently, small temperature non-uniformities at the optical windows appear as a distinct background. Comparatively, the CMT schlieren setup is less affected by background inhomogeneities. Nevertheless, high-temperature combustion gradients of the spray are easily measured. Further details regarding the CMT schlieren setup are found in Refs. [15, 22]. Recent changes to the Sandia schlieren setup have increased the light source aperture from 1 mm to 3 mm to reduce the effect of background inhomogeneities [4].

Table 2. Specifications of the optical diagnostics employed

	Broadband chemiluminescence	Sandia schlieren	CMT schlieren
Camera	Phantom v7.1 CMOS	Phantom v7.1 CMOS	Photron SA-5 CMOS
Lens	Nikon 50 mm (f/1.2)	Nikon 85 mm (f/2.8)	Nikon 50 mm (f/1.8)
Filter	600 nm short-pass	450 nm band-pass	360 - 580 nm band pass
Exposure	46 μs	10 μs	4 μs
Framing Period	50 μs	26.25 μs	23.8 μs
Resolution	512 x 128	400 x 112	576 x 224
Light Source	-	450 nm LED	Xenon lamp
Source Aperture	-	1 mm diaphragm	1 mm diaphragm
Stop Aperture	-	none	4 mm diaphragm

1-D TRANSIENT GAS-JET MIXING-CHEMISTRY MODEL

To aid in the interpretation of the experimental trends and to further probe the coupling between mixing and chemistry during end-of-injection, a recently developed 1-D transient gas-jet mixing-chemistry model, is used [23]. Building on recent developments of a 1-D transient gas-jet mixing model [24], which is capable of predicting transient jet penetration and mixture fraction distribution, the current model also solves chemical kinetics in each control volume. A graphical representation of this model is shown in Figure 3.

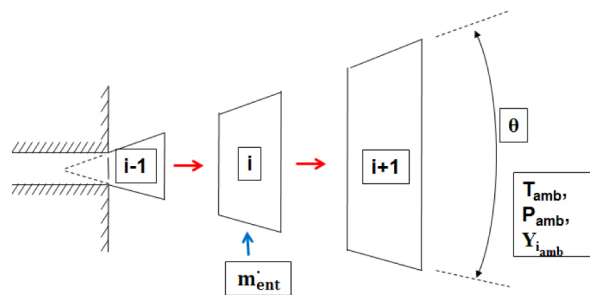


Figure 3. 1-D transient gas-jet mixing-chemistry model. More details are found in [23].

The 1-D transient gas-jet mixing-chemistry model is composed of a series of discrete control volumes, positioned axially along the jet axis. The volume of each control volume is determined *a priori* by a

user-supplied constant spreading angle, θ , of the jet. Fuel mass and momentum conservation equations are solved numerically in each control volume, i , to obtain the ambient entrainment rate, $\dot{m}'_{\text{ent}}$, for an arbitrary injection profile. To incorporate chemistry predictions, species and energy conservations equations are then solved for each control volume with the previously found ambient entrainment rate as an additional influx. For example, control volume i takes in mixtures from $i-1$ and the ambient, as specified by the ambient entrainment rate. The mixture within control volume i then undergoes adiabatic mixing and is allowed to react, at constant pressure, for the duration of the residence time. The control volume is considered a well-stirred reactor, i.e. no sub-grid turbulent combustion model is used. Note that simulations begin at start-of-injection and terminate 6 ms later, allowing sufficient simulation time to capture ignition as well as the possibility of combustion recession.

One key feature of the 1-D transient gas-jet mixing-chemistry model is that simultaneous mixing and chemistry can be realized. Mixing alone is not sufficient to understand complex ignition processes during transients, i.e. at the end-of-injection. Chemistry predictions are modeled with the aid of the reduced dodecane mechanism of Wang et al. [26], consisting of 100 species and 432 reactions. Predictions of mixture fraction and jet penetration agree well with experimental measurements of ECN Spray A and H [25]. Ignition timing has also been validated for Spray H [23]. While the fluid mechanics are highly simplified, this approach captures the main mixing features of the jet. Therefore, another key feature is that computational resources are reserved for comprehensive chemical mechanisms that would otherwise be intractable in higher-fidelity 2-or 3-D RANS and LES codes. While the model is capable of handling large chemical mechanisms, the large number of simulations performed in the current work prompted the use of a moderately reduced mechanism [26].

DESCRIPTION OF COMBUSTION RECESSION BASED ON MEASUREMENTS AND 1-D MODEL

High-gain chemiluminescence and high-sensitivity schlieren images, acquired simultaneously during the same injection for a temperature variation on the Spray A condition, are shown in Figure 4. While these still images do not best convey the transient nature of combustion recession, the movies for each condition are provided at Ref. [27] for the benefit of the reader. The gain is increased in all of the chemiluminescence images to show the weak signal in the region between the nozzle and the lift-off length (shown as the most upstream location of the blue contour). The threshold for saturation (shown in red) is set to 50% of the intensity at the mean lift-off length. Times listed are after start-of-ramp-down (aSORD).

Focusing on the 1000 K condition, evidence of strong combustion recession is observed. By 209 μs aSORD, injection has completely ended. Upstream of the lift-off length (12 mm from the injector), the jet imaged by schlieren has become transparent and no luminosity is observed in the chemiluminescence images, indicating that liquid fuel has completely vaporized and that these regions have reached a temperature similar to the ambient environment. This indicates that

cool flame reactions have taken place throughout these mixtures. Again, the reader is encouraged to view the movies at Ref. [27] frame by frame to more clearly see these end-of-injection processes.

Suddenly, at 259 μs aSORD, chemiluminescence appears upstream of the quasi-steady lift-off length, to approximately 7 mm from the injector, indicating the beginning of high-temperature reactions in the upstream mixtures, or combustion recession. Similarly, the schlieren image at 271 μs aSORD shows a simultaneous darkening and softening in image texture upstream of the quasi-steady lift-off length in the same location. This change in texture is due to large gradients in the refractive index from high-temperature combustion products. The schlieren images and movies in Refs. [4] and [28] also show evidence of high-temperature combustion, and combustion recession, but these setups yield more dark contrast at high-temperature combustion zones rather than a soft texture. By 309 μs aSORD, the simultaneous chemiluminescence/schlieren images show that combustion has recessed to its furthest observable upstream location, approximately 2-3 mm from the injector. High-temperature chemiluminescence decays in time, while high-temperature products remain, as indicated by the index-of-refraction gradients still visible in the schlieren images. Throughout the period where high-temperature ignition reactions are observed to occur in the upstream mixtures, the combustion appears as though it were a backward traveling wave. Such an observation could suggest that this combustion recession is driven by flame propagation through the upstream mixtures as injection velocities decline. However, as discussed later, the speed of this recession is much faster than turbulent flames speeds under these conditions, suggesting that the combustion recession is more indicative of a sequential recession of ignition reactions back towards the injector [4].

By 509 μs aSORD, strong luminosity is observed near the injector and is likely from soot luminosity. Soot formed at this instance is likely due to combustion of end-of-injection dribble, which forms large poorly mixed pockets of fuel as shown by high-speed microscopy performed at the exit of the nozzle [29]. This natural soot luminosity signal consistently occurs for cases with combustion recession but it appears with a more random delay after the end of injection, presumably because of the timing of the dribble event. We verified that the signal was from soot luminosity, rather than from Mie-scatter from droplets, by demonstrating that the signal remained the same with and without laser illumination to the region (see movies at [20]).

The first frame of the chemiluminescence images (44 μs aSORD) for the 900 K ambient condition is during the injection ramp down process and shows liquid droplets still exiting the nozzle. The droplets are visible because emission from downstream soot incandescence is elastically scattered from the liquid droplets. The first evidence of combustion recession appears at 444 μs aSORD in the chemiluminescence images and is noticeably weaker than the 1000 K condition. In contrast to the 1000 K case, the luminosity upstream of the flame lift-off length (now at ~ 16 mm) at 444 μs aSORD shows pockets of ignition receding back towards the injector instead of a connected backward traveling wave. The pockets are also evident in the schlieren images, first at 463 μs aSORD, which later merge as time progresses. Both diagnostics used cautioning

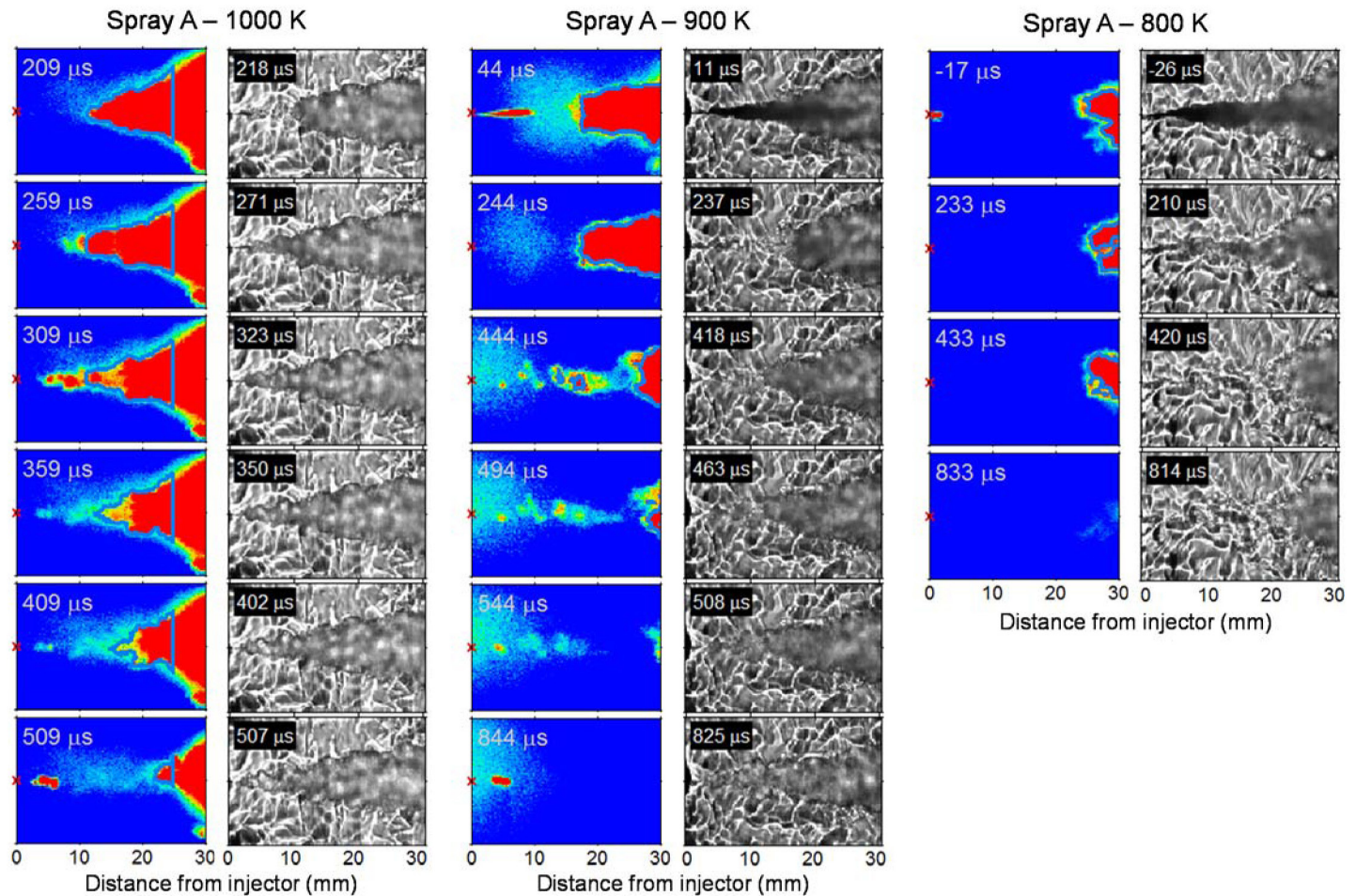


Figure 4. Simultaneously captured chemiluminescence and schlieren images of combustion recession for a temperature variation on the ECN Spray A condition. Images were acquired at Sandia.

the observed ignition pockets at the 900 K ambient condition are indeed separated ignition sites. This transition from a sequential combustion recession at 1000 K to pockets of separated ignition sites at 900 K further suggests that the reactions under both conditions are driven by autoignition rather than flame propagation. Lastly, soot luminosity of burning dribble is again noticeable at 844 μ s aSORD.

In contrast to the higher ambient temperature conditions, the 800 K condition shows no evidence of combustion recession in either the chemiluminescence or schlieren images. Also, because there is a lack of soot incandescence at this low ambient temperature, no Mie scatter from liquid droplets is observed near the injector at -17μ s aSORD even through the injection event has not yet ended. Based on these images, it can be seen that ambient temperature plays a significant role in determining the likelihood of combustion recession.

In order to better understand the nature of combustion recession and how each diagnostic may measure different features of the combustion recession process, the 1-D transient gas-jet mixing-chemistry model is employed in the following discussion. In the model, the end-of-injection ramp-down process is modeled as a linear decrease of injection velocity with time that occurs over a duration of 100 μ s, which is consistent with the experimentally measured ramp down duration for the injectors used in this study (see Figure 2).

While the inherent 1-D nature of the model prevents spatially accurate predictions of LOL, the trends of predicted ignition delay and LOL with ambient temperature are consistent with experimental results, as shown in Table 3. The results in Table 3 show that the 1-D model over-predicts LOL by 50-60%, while ignition delays are over-predicted by 30-45%. Though ignition and lift-off processes are not uncoupled, accurate prediction of ignition processes are likely to be more important for capturing the physics of combustion recession.

Table 3. Comparison of experimental and model predicted ignition delays and flame lift-off lengths.

Ambient temperature (K)	Exp. ignition delay (ms)	Model ignition delay (ms)	Exp. flame lift-off length (mm)	Model flame lift-off length (mm)
800	0.85	1.1	26.2	39
900	0.44	0.65	16.5	28
1000	0.24	0.35	12.2	19

Figure 5 shows the time history of equivalence ratio and temperature from a computational cell within the jet located 1 mm from the injector, at four different ambient gas temperatures. This region is