Investigation on the use of unsteady flamelet modeling for transient diesel spray combustion processes

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Abstract
This study seeks to explore the use of unsteady flamelet modeling in the numerical simulation of steady-state flame development and combustion recession in a chemically reacting diesel spray following an end-of-injection transient. The heterogeneous mixture formation in sub-grid scale and turbulence-chemistry interaction are modeled with the use of a Representative Interactive Flamelets (RIF) model. The RIF model has been incorporated with a Eulerian Particle Flamelet Model (EPFM) approach that employs multiple flamelets to leverage the unsteady flamelet history. The results are compared against a first-order moment method, i.e. Well-Stirred Reactor (WSR) model. The simulations have been performed with a Reynolds Averaged Navier-Stokes (RANS) framework incorporated within the commercially-available CFD code, CONVERGE. The present study demonstrates the prediction capability of two combustion models, and characterizes the predicted ensemble-averaged turbulent mean scalars in comparison to experimental observations from the Engine Combustion Network (ECN). Detailed analysis of simulations employing varying number of flamelets in the RIF-EPFM approach reveal some artificially induced combustion instabilities that manifest as an oscillatory behavior of the flame lift-off length. This instability is found to be alleviated by properly tracking flamelet scalar-dissipation-rate history; i.e. further increase of flamelets attenuate the oscillations in reaction zone. Moreover, it is shown that the use of flamelet model better captures the experimentally observed end-of-injection combustion, so-called combustion recession in terms of ensemble-averaged turbulent mean quantities of reaction zone.

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Introduction

Modern advanced combustors often encounter multi-physics problems involving simultaneous occurrence of multi-phase turbulent mixing, heat transfer, and chemical reactions. The intrinsic complexity of the problems generally brings non-linear nature that makes deterministic solution prohibitively limited in reduced dimensional analysis. One of the important challenges encountered in designing future-generation clean combustion engine is subject to understanding of interactive turbulent-chemistry process. Therefore, it is very demanded to facilitate various ranges of turbulent combustion studies over relevant engine operating conditions. In this context, many research groups have devoted great amount of experimental and computational studies and their experiences to Engine Combustion Network (ECN) [4], which enables to provide a worldwide collaborative platform for engine combustion studies.

In the meantime, the highly non-linear and multi-scale nature of diesel engine combustion gives very limited allowance to deterministic analysis. Of many modeling strategies, difficulty in turbulent combustion modeling has particularly been emphasized because turbulent-chemistry interaction (TCI) is very likely to dominate unsteady flame stabilization, auto-ignition/quenching as well as pollutant formation process. Recently, various TCI modeling strategies [3,12-14] have been examined and assessed against homogeneous mixture combustion model, i.e. well-stirred reactor (WSR) model. The WSR model is characterized by its explicit modeling, so it directly integrates the rate of change in species concentration with simplification of homogeneous charge of mixture over a computational grid scale. This approach of direct integration subsequently neglects the contribution of turbulent fluctuations in mixing field and reacting scalars, which otherwise plays a significant role in determining chemical reaction rate.

Over the last decades, many of turbulent combustion modeling approaches have been developed to take finite-rate of chemistry into account. When it comes to the non-premixed diffusion flame in particular, the laminar flamelet model [15] has been popularly used due to its less demanding computational cost, which is achieved by transforming three-dimensional physical space into one-dimensional reaction space, i.e. mixture fraction. This approach benefits one-dimensional flamelet equation with no presence of non-linear convective term. Moreover, since the complex chemistry should be incorporated in the reaction space instead of being present in the species conservation equations, the CFD time step no longer accounts for stiff chemical time scale change, therefore the computation may remain more stable and potentially faster. The coupling between physical space and reaction space is then achieved by introducing local instantaneous scalar dissipation rate, \( \chi \), that represents the local molecular mixing intensity across the thin layer of reaction zone.

Basic idea of the flamelet model is to view a turbulence diffusion flame in mixing field as an ensemble of laminar stretched diffusion flames locally embedded in a turbulent mixing field. The first attempt of this approach was introduced by Peters [15] and it constructs a steady-state flamelet library that computes reactive scalars as only a function of mixture fraction, \( Z \), referred to as Steady Laminar Flamelet Model (SLFM). The SLFM approach was later extended to unsteady turbulent combustion problem by reformulating the flamelet equation with introduction of two independent flamelet parameters, i.e. \( Z \) and \( \chi \). Pitsch et al. [18] later emphasized the importance of unsteady effects particularly in slow chemical kinetics and proposed so-called Representative Interactive Flamelets (RIF) model [16]. The RIF model basically inherits the basic idea of flamelet model in its stand-alone flamelet solver, which communicates with the CFD solver at each CFD time step. The flamelet parameter that links the global turbulent mixing field is incorporated as a nominally averaged scalar dissipation rate conditioned over the stoichiometric mixture. They further showed successful capability of evaluating turbulent mean quantities with presumed probability density function (PDF) along with the flamelet solutions under various engine relevant conditions. [17].

In the past decades, demands for next-generation clean and energy-efficient diesel engine combustion have drawn many concerns regarding increasingly strict emission regulations. Despite superior thermal efficiency of diesel engine, controlling the emissions of nitrogen oxide (NOx) and particulate matters remain questioned with conventional diesel combustion techniques. In this regard, low-temperature combustion (LTC) technique has received great attentions among many combustion groups, and they have revealed potentials of low NOx alternatives [5,9]. In the meantime, the LTC techniques have faced another issues related to unburned hydrocarbon (UHC) and carbon monoxide (CO) emissions subject to incomplete combustion. Recent experimental [8,9,11] studies have demonstrated that major part of the UHC and CO emissions are associated with the transient nature of diesel injection. Very recent studies [6,7] have also qualitatively identified transient flame dynamics that promotes complete consumption of UHC after end-of-injection (EOI) and referred it to as combustion recession. This finding motivated us to explore further analysis on the evolution of thermo-chemical properties of spray mixtures during this end-transient period.

This study seeks to examine the impact of turbulent-chemistry interaction in capturing steady and transient diesel combustion dynamics. In this context, this
study aims to further understand the role of turbulent mixing in evaluation of turbulent mean reactive scalars, and examine the intrinsic characteristics of RIF model in comparison to the WSR model approach.

**Numerical Formulations**

Balance equations for all conserved variables for turbulent mixing field are constructed in a Reynolds-Averaged Navier Stokes (RANS) framework. To avoid complexity that may arise when evaluating turbulent mean quantities associated with compressible flow, the Reynolds-averaged quantities are formulated with adopting Favre average operator \( \bar{\phi} \) with any primitive variable \( \phi \).

To construct the statistics of turbulent mixing field, mean quantities of additional conserved scalars, first and second-order moments of mixture fraction, should be determined along with RANS solution.

\[
\frac{\partial \bar{Z}}{\partial t} + \frac{\partial \bar{U}_i \bar{Z}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \bar{\rho} \frac{\partial \bar{Z}}{\partial x_i} \right) \tag{1}
\]

\[
\frac{\partial \bar{Z}^2}{\partial t} + \frac{\partial \bar{U}_i \bar{Z}^2}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \bar{\rho} \bar{u}_i \bar{Z} \right) + 2\bar{\rho} \left( -\bar{\nu}_i \bar{Z} \right) \frac{\partial \bar{Z}}{\partial x_i} - \bar{\rho} \chi \tag{2}
\]

where,

\[
\chi = c_\chi \frac{\bar{Z}^2}{k} \tag{3}
\]

Note that the molecular diffusive transport terms have been neglected for simplicity assuming high Reynolds turbulent flow. Turbulent transport terms formulated as higher moments of turbulent fluctuations are modeled with gradient transport assumption, where the turbulent diffusivity is determined with presumed turbulent Schmidt number, \( S_c \): \( D_t = \nu_t / S_c \), where \( \nu_t \) is turbulent viscosity that is determined from the employed turbulent model for RANS framework. It is also important to emphasize that the mixture fraction variance equation in Eq. (2) introduces the role of turbulence present in local mixing intensity and is constructed with similar form of turbulent kinetic energy transport equation. Therefore, it indicates that the scalar dissipation rate appearing in the last term plays an equivalent role of turbulent kinetic energy dissipation rate, \( \varepsilon \). However, it should also be noted that the scalar dissipation rate generally happens in very small time and length scales, so it is very hard to directly evaluate the quantity from the RANS solution. In general, this quantity is modeled by utilizing the known turbulence quantities, i.e. turbulent kinetic energy, \( k \), and its dissipation rate \( \varepsilon \) in Eq. (3). Here, \( c_\chi \) is a free parameter that typically employs 2.

**Chemistry Closure Modeling**

In this study, we examine two different approaches of combustion closure problem: Well-Stirred Reactor (WSR) model and Representative Interactive Flamelets (RIF) model. The WSR model is incorporated in CONVERGE code [19] in the name of SAGE model and treated as a part of the CFD solution, whereas the RIF model needs to be handled with separated stand-alone 1-D flamelet solver. We employed multiple flamelet model approach in support of Eulerian Particle Flamelet Model (EPFM).

**Well-Stirred Reactor (WSR) model**

The WSR model directly quantifies the species production rate appearing as a source term in the species transport equations, i.e. \( \bar{\omega}_k \), in the species transport equations. Rather than accounting for heterogeneous nature of mixture formation in computational grid scale, it computes the reaction rate directly from the mean reactive scalars based on Arrhenius law formulation, \( \dot{f}_k(Y, T) \), neglecting high order non-linear impact of turbulent fluctuations. Accordingly, it simply expresses the integration of function of mean temperature and mean species mass fractions in Eq. (4). In most turbulent combustion applications, however, this approximation may yield errors by several order of magnitude because of the intrinsic non-linear nature of the Arrhenius law formulation.

\[
\bar{\omega}_k = f(Y_k, T) \tag{4}
\]

**Representative Interactive Flamelets (RIF) model**

The RIF model benefits from the coordinate transformation from three-dimensional physical space to one-dimensional reaction space. It enables to separate the chemistry computation from the CFD solution. The basic assumption lies in the laminar flamelet concept, which views a turbulent diffusion flame as an ensemble of locally undisturbed laminar diffusion flamelets. This approach holds for very thin layer of reaction zone, and consequently substantial scalar gradient is assumed to be normal to the flamelet surface. The resulting formulation of reactive scalars, e.g. \( k \)-th species mass fraction, \( Y_k \), to express the inner structure of laminar diffusion flame is therefore formulated as:

\[
\rho \frac{\partial Y_k}{\partial t} = \omega_k + \frac{1}{2} \rho \bar{\nu}_i \frac{\partial^2 Y_k}{\partial Z^2} \tag{5}
\]

where the scalar dissipation rate is evaluated by square of mixture fraction gradient:

\[
\chi = 2 \bar{D} \left( \frac{\partial Z}{\partial x_i} \right) \tag{6}
\]

The importance of the scalar dissipation rate in Eq. (6) is that it couples the mixing field and local flamelet structure and it is characterized by the inverse of molecular diffusion time scale. In the counterflow diffusion flame problem for example, the scalar dissipation rate is an indicator of flamelet strain rate. For this rea-
son, the scalar dissipation rate can be considered as an eigenvalue for unsteady flamelet quenching and autoignition problem.

Another essential feature of the RIF model is achieved by the statistical description of turbulent mixing field with random variable of mixture fraction, $Z$. The turbulent mean reactive scalars, $Y_e$, in physical space is thus determined by the first moment of instantaneous scalar, $Y_{e_i}$, from the reaction space using a presumed shape of PDF in Eq. (7). We employed the beta PDF expressed in Eq. (8) for the present RIF simulations.

$$\tilde{Y}_e(x,t) = \int_0^1 Y_e(Z,t) P(Z, \tilde{Z}, \tilde{Z}^2; x,t) d\tilde{Z}$$  \hfill (7)

$$P(Z, \tilde{Z}, \tilde{Z}^2; x,t) = \frac{Z^{\alpha - 1}(1 - Z)^{\beta - 1}}{\Gamma(\alpha)\Gamma(\beta)} \Gamma(\alpha + \beta)$$  \hfill (8)

where $\alpha = \tilde{Z}\gamma$, $\beta = (1 - \tilde{Z})\gamma$, and $\gamma = (1 - \tilde{Z})/\tilde{Z}^2 - 1$.  

**Eulerian Particle Flamelet Model (EPFM)**

Use of single flamelet library is known to have deficiency in highly unsteady turbulent diffusion flame because domain averaged scalar dissipation approximation may not properly reflect the small-scale local mixing and resulting unsteady nature. Baths et al. [1,2] suggested the concept of multiple flamelets to account for temporally varying flamelet history in space. In this approach, the mass weighted fraction of Eulerian particles is tracked as markers solution of corresponding flamelet, and constructed as conserved scalar equation form identically with the mean mixture fraction equation in Eq. (1). The fraction of markers over the total mixtures can be denoted as $Z_i$, for $i$-th flamelet. Due to the turbulent mixing process, different Eulerian markers from different flamelet may be collocated, therefore the solution should satisfy the following condition:

$$\tilde{Z} = \sum_{i=1}^N \tilde{Z}_i$$  \hfill (9)

where $N$ is the total number of flamelets. Alternatively, the probability to find a marker corresponding to $i$-th flamelet out of all other flamelets is often denoted as $T_i = \tilde{Z}_i/\tilde{Z}$. Accounting for this additional dependence, the Eq. (7) should be recast being weighted by $T_i$. The detailed formulation is not repeated for the sake of brevity.

**Test Methodology**

In this study, several RANS simulations of diesel spray combustion have been conducted under both non-reacting and reacting conditions. The spray model and grid convergence have been tested and tuned against the vaporizing spray experiment [4] based on ECN Spray A conditions. The Spray A condition replicates spray injection and in-cylinder ambient conditions encountered in diesel engine operation. Spray A injector is equipped with a single-hole axially-drilled orifice. The fuel is injected into a quiescent gas within a cubic-volume test chamber (10 x 10 x 10 cm$^3$) and freely evolves in the chamber. Details of the specific test conditions adopted for the present simulations are summarized in Table 1. The ECN nominal Spray A mass flow rate was borrowed from the ECN website for the spray boundary condition and its duration was set to 1.5 ms. We also specify that the start of the end-of-injection (EOI) ramp-down profile begins at 1.46 ms.

<table>
<thead>
<tr>
<th>Test type</th>
<th>Reacting flow</th>
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<tbody>
<tr>
<td>Fuel</td>
<td>n-dodecane (C$<em>{12}$H$</em>{26}$)</td>
</tr>
<tr>
<td>Nozzle diameter [µm]</td>
<td>90</td>
</tr>
<tr>
<td>Fuel temperature [K]</td>
<td>363</td>
</tr>
<tr>
<td>Injection duration [ms]</td>
<td>1.5</td>
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<tr>
<td>Injected fuel mass [mg]</td>
<td>3.5</td>
</tr>
<tr>
<td>Injection pressure [MPa]</td>
<td>150</td>
</tr>
<tr>
<td>Ambient gas temp. [K]</td>
<td>900</td>
</tr>
<tr>
<td>Ambient gas composition [by vol.]</td>
<td>O2: 15%, N2:75.15%, CO2: 6.23%, H2O: 3.62%</td>
</tr>
</tbody>
</table>

**Table 1.** Test conditions for ECN Spray A [4]

![Computational grid setup with adaptive mesh refinement (AMR)](image)

The present simulations have been performed with the finite volume method CFD code platform, CONVERGE [19]. The code is capable of constructing a structured mesh with static and dynamic mesh refinement; i.e. adaptive mesh refinement (AMR). The AMR has been utilized in regions where any of the user-specified thresholds for fuel mass fraction (10$^{-5}$), or OH mass fraction (10$^{-6}$) are reached. The base grid scale was set to 4 mm and the smallest grid scale allowed via 4 levels of AMR was 0.25 mm as shown in Figure 1.

**Results and Discussions**

The main focus of this study lies on exploration of TCI modeling effect on predictions of steady-state and transient turbulent spray flame. In pursuit of this goal, we have validated our spray model setup against the
ECN experiment, which are not listed in this paper for brevity. Based on the model validity, we further explore the impacts of TCI modeling on prediction of turbulent mean profile and general characteristics of the lifted diesel spray flame. Finally, we will discuss the model accuracy achieved when simulating transient combustion recession phenomena.

Steady-State Spray Flame Development

Figure 2. Quasi steady-state flame at TASoI (Time after start of injection) = 1.46 ms. White solid line in Z contour: iso-stoichiometric mixture, White solid line in OH contour: OH level at 2% of maximum steady-state concentration. Use of 20 flamelets for RIF model as suggested for Spray A by Kundu et al. [10]

In this section, we examine several important features of approximated turbulent mean scalar fields produced by the TCI modeling. One of the important aspects of turbulent combustion physics is its intermittency characteristic. In practical turbulent flows, this is often encountered with unsteady nature of flapping flame brush, which in turn should exhibit rather distributed transverse profile when ensemble-averaged. Therefore, the key principle of the TCI modeling is to approximate turbulent “mean” flame profile rather than capturing instantaneous laminar profile especially in RANS framework.

Figures 2 (A) and (b) illustrate quasi-steady lifted flame captured at TASoI = 1.46 ms, shortly before the EOI transient begins. One can see different OH profiles across the spray flame periphery, whereas the mixture fraction field looks rather qualitatively similar. It is important to notice that the RANS resolved OH mass fraction field with RIF model reveals substantially thick profile of numerical solution, whereas the WSR model estimates non-zero level of reaction in the vicinity of stoichiometric mixture with much narrower span. Also the approximated OH field with RIF model seemingly shows lower peak of OH level across the stoichiometric line. This implies that the introduction of PDF in RIF model gives rise to a broader mean reacting scalar profile, and consequently a more dissipative solution. Such a rather distributed flame profile by the RIF model support the idea of intermittency captured by the TCI modeling, because highly unsteady turbulent feature of spray flame may intermittently sweep over a broad range of physical space such that its ensemble-averaged quantity no longer exhibit sharp change in reaction zone.

Effect of TCI modeling on unsteady turbulent combustion dynamics

Figure 3. Temporal change of maximum temperature with different flamelet setups

Diesel spray combustion is in general characterized by an outcome of finite rate of chemistry along with turbulent mixing process. As a result, the flame is very likely to initiate a certain amount of time after injection begins and settle down at a certain distance from the injector. Here we determine the ignition delay time (ID) and flame lift-off length (LOL). Those metrics are commonly employed for assessment of modeling accuracy against experimental data. A very widely adopted method to determine ID is based on temperature rise; i.e. the ECN recommended that ID be measured at the time instance of maximum rate of maximum temperature within the computational domain. The LOL is defined to be the length from the injector to the axial position of 2% of maximum steady-state Favre averaged OH mass fraction.

Questions may arise when the maximum rate of temperature rise is not straightforwardly defined. Figure 3 exemplifies the situations that use of multiple flamelets with RIF model makes a rather gradual increase of maximum temperature. For RIF model with 30 flamelets, the LOL may be sensitively determined over a wide range of time (0.5 ~ 1.0 ms), whereas one can find evident peak rate of temperature rise in the case of WSR model and some cases with small number of flamelets.
This limitation motivated us to find an alternative way for evaluating ID. The ECN also suggested to measure the ID based on OH level in the same way that the LOL is determined; therefore, the ID can be determined as the first time at which Favre-average OH mass fraction reaches 2% of the maximum in the domain after a stable flame is established. Figure 4 illustrates the tendency of ignition delay time according to the number of adopted flamelets in the RIF model. Although earlier study [10] stated that the prediction accuracy would become better as the number of flamelets increases, the best accuracy in the ID was achieved with 10 flamelets and the calculated ID seems to settle at around 0.6 ms as the flamelet number keeps increasing.

As found in an earlier study [10], the use of RIF model with multiple flamelets produces the oscillatory behavior of flame dynamics as reproduced in Figure 5. To further look into this issue, this section revisits the details of unsteady behavior of the flamelet solution with various multiple flamelets condition. Figures 5 (a-f) sweep different choice of flamelet numbers and the WSR model, and illustrates the temporal change of flame lift-off length (LOL), flame length (FL) which is the furthest position of reaction zone, and domain integrated heat release rate (HRR). The LOL and FL were evaluated by the OH mass fraction base method. The present simulations have reproduced the previously reported oscillatory behavior in LOL and HRR with the RIF model set-up; however, the flame length was very similar regardless of the flamelet number. Therefore, further analysis needs to be made focusing on the region where the lifted flame settles down. This will be discussed in the following section.

**Figure 4.** Effects of number of flamelets on ignition delay time based on OH mass fraction trace.

**Figure 5.** Temporal variation of flame lift-off length (LOL), flame length (FL), and domain integrated heat release rate (HRR): Observation of oscillatory behavior in flamelet represented solution. The quantities of LOL and FL were evaluated at 2% of maximum OH mass fraction.
Overall characteristics of diesel spray combustion is observed consistently over the various model set-up except for single flamelet model set-up; i.e. success of capturing lifted diesel spray flame has solely been made by the RIF model with finite number of flamelets and the WSR model. In addition, the combustion recession is also identified by observing shortened LOL during the end-of-injection (EOF) period; i.e. after 1.46 ms. However, the single flamelet set-up failed to settle the lifted flame downstream; i.e. once the very initial reaction occurs downstream at around 30 mm, the LOL then rapidly recess back towards the injector. In addition, the single flamelet solution does not exhibit the oscillatory behavior in LOL and HRR variations. The primary reason is that the scalar dissipation rate, $\chi$ in Eq. (5) was determined by domain-averaged value over the entire space that the spray mixture occupies. Therefore, the domain-averaged value of $\chi$ may not convey the impact of locally intensive turbulent mixing particularly near the injector location. Consequently, it is very likely that the local quenching due to high scalar dissipation rate was prohibited in the upstream field.

On the other hand, all other solutions from multiple flamelets present the oscillating flame dynamics between the nozzle and the LOL. It is also important to note that the oscillations are observed at consistent frequency of flamelet initiation; e.g. there are five peaks of HRR and LOL with 5 flamelets set-ups shown in Figure 5 (c). Then, the oscillation amplitude is attenuated with further increase of flamelet number. Thus, this gives strong implication that distinct RIF solution from the subsequent flamelet libraries may cause the discontinuous solution of reactive scalars.

Figure 6 (a) further illustrates the moment at which the significant oscillatory peak appears. The sudden change in OH mass fraction also indicates discontinuous combustion process at the moment. This observation can be explained by identifying the individual RIF solution represented by each of flamelet libraries, and Eulerian marker solution $Z_t$ limits the spatial domain where the corresponding flamelet solution covers. It should also be emphasized that different Euler marker solutions may overlap together due to turbulent mixing; therefore, each of flamelet solutions is weight-averaged to determine resulting turbulent ‘mean’ value. Based on this idea, the sudden expansion of spray flame area found at 0.66 ms provides an evidence that the second flamelet solution has finally contributed its ignition phase to the turbulent mean quantity; consequently, yielding rapid increase of OH species production.

Figure 6 (c) presents temporal variations of domain-averaged scalar dissipation rate for each of flamelet libraries. Each flamelet is initiated at uniform time intervals out of injection duration, and encompasses a certain portion of injected fuel amount and domain occupation indicated by Eulerian marker solution. Based on this observation, the idea that the scalar dissipation rate can be considered as an eigenvalue for unsteady quenching and auto-ignition seems to hold for the present simulation. Knowing that the ignition delay time (ID) should be captured by the first flamelet solution and was found at 0.45 ms from Figure 4, the eigenvalue of $\chi$ for flamelet solution to ignite can be evaluated at around 13 as indicated with black dashed line in Figure 6 (c). The concept of the eigenvalue problem for local auto-ignition is supported by finding that the second flamelet’s scalar dissipation rate meets this value at the time instance of 0.65 ms at which we observed the noticeable ignition contribution by 2nd flamelet; i.e. oscillatory peak, in Figure 6 (a).
**Combustion Recession**

This section focuses on the predicted end-of-injection (EOI) combustion transient; i.e. combustion recession. The left column of snapshots in Figure 7 shows instantaneous images of OH chemiluminescence from ECN experiments [4], and the right two columns are RANS solutions with the WSR model and the RIF model. Prior experiments by Knox and Genzale [6,7] have identified distinctive combustion recession regimes at different ambient thermodynamic conditions. They observed weak or partial combustion recession regime at our test condition; i.e. T = 900K. This specific combustion regime shows very clear indications of separated small-scale pockets of ignition upstream of the lift-off length as revealed in ECN chemiluminescence images in Figure 7. It is noted that the RANS solution is very limited in capturing experiment-like instantaneous features. Rather the present RANS data only demonstrates the likelihood of combustion recession. In this context, although the WSR model predicts the occurrence of combustion recession, it does not extend very far upstream where high OH regions are observed in the experiment. A possible reason is that the first order moment method cannot accommodate the small-scale heterogeneous mixing and reactions in sub-grid scales. However, the RIF model predicts a much more elongated combustion recession zone, covering up to the near nozzle location, which is more consistent with the experiment. It implies that the RIF model captures combustion recession in the vicinity of injector consistent with the experiments.

![Figure 7. Occurrence of combustion recession: Instantaneous snapshots from ECN experiment (left first column) and ensemble averaged OH mass fraction from the present simulations. The spray flame boundary is detected at 2% of maximum steady-state maximum OH level. Time indicates the elapsed time after start of injection ramp-down.](image)

**Conclusions**

We conducted RANS simulations with two different combustion modeling: WSR vs. RIF. The RIF model was incorporated with multiple flamelets approach such that unsteady history of flamelet solution is well captured. Important findings from the present study is summarized as follows:

1. Since the WSR model excludes the non-linear effect that accommodates the sub-grid scale heterogeneous mixing, it produces a laminar reaction profile in the mixture fraction field; so its RANS solution exhibits a thin reaction zone across the stoichiometric mixture line.

2. The RIF model with multiple flamelets can predict the finite rate of reaction progress and lifted spray flame. Moreover, the incorporation of presumed PDF when determining turbulent mean scalar field is capable of predicting the intermittency effect, which accounts for unsteady turbulent motion that determines the turbulent mean value. Accordingly, the prediction shows a wider reaction zone and lower peak OH concentration compared to those of WSR model prediction.

3. Despite the accomplishment of turbulent mean profile, the RIF model may accommodate undesirable numerical artifacts that exhibit oscillatory behavior in reacting zone. This may be subject to the inaccurate realization of unsteady flamelet history and limitation of finite number of flamelet libraries. However, increasing the number of flamelets can attenuate the oscillatory behavior.

4. Two different combustion models, WSR and RIF, well captured combustion recession. Even though the ensemble averaged solution from the RANS framework is rather prohibited from obtaining instantaneous features of combustion transient, the RIF model seems to better follow the qualitative characteristics of combustion recession behavior, which is experimentally observed. On the other hand, the WSR model failed to capture the likelihood of appearance of weak/partial combustion recession regime at the current test condition.

**Abbreviations**

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tr>
<td>ECN</td>
<td>Engine Combustion Network</td>
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<tr>
<td>EOI</td>
<td>End of Injection</td>
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<tr>
<td>EPFM</td>
<td>Eulerian Particle Flamelet Model</td>
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<tr>
<td>ID</td>
<td>Ignition Delay</td>
</tr>
<tr>
<td>LOL</td>
<td>Lift-Off Length</td>
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<tr>
<td>LTC</td>
<td>Low Temperature Combustion</td>
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<tr>
<td>PDF</td>
<td>Probability Density Function</td>
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<tr>
<td>TSoI</td>
<td>Time after Start of Injection</td>
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