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# Modeling the ignitability of a pilot injection for a Diesel Primary Reference Fuel: impact of injection pressure, ambient temperature and injected mass

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# Abstract

In this paper, we studied the accuracy of computational modeling of the ignition of a pilot injection in the Sandia National Laboratories (SNL) light-duty optical engine facility, using the physical properties of a cetane/iso-cetane Diesel Primary Reference Fuel (DPRF) mixture and the reaction kinetics of a well-validated mechanism for primary reference fuels. Local fuel-air equivalence ratio measurements from fuel tracer based planar laser-induced fluorescence (PLIF) experiments were used to compare the mixture formation predictions with KIVA-ERC-based simulations. The effects of variations in injection mass from 1 mg to 4 mg, in-cylinder swirl ratio, and near-TDC temperatures on non-combusting mixture preparation were analyzed, to assess the accuracy of the model in capturing average jet behavior, despite its inability to model the nonnegligible jet-by-jet variations seen in the experiments. Fired simulations were able to capture well the measured ignitability trends at the different injection conditions tested, but showed some deviations in the minimum temperature needed for robust ignition, pointing out the need for further work to focus on achieving fully comprehensive modeling with detailed chemical kinetics of the DPRF58 mixture and a full engine geometry representation.

# Introduction

Usage of pilot injection strategies in diesel engines operated with conventional diesel combustion (CDC) modes is widely adopted in order to reduce the delay of the main ignition event, smoothen the premixed combustion phase and consequently reduce noise and pollutant emissions at partial loads [1-4]. However, more advanced and low-temperature compression ignition combustion strategies typically feature early injections and high charge dilution levels achieved by means of high exhaust gas recirculation (EGR) rates. Here, the benefits of adding pilot injection stages before the main injection can be difficult to achieve and are still not well understood. In fact, small pilot quantities may fail to ignite when the local charge conditions are too dilute or temperatures are too low, and robust ignition may be re-established by increasing the pilot injected mass, at the price of compromising the emissions performance of the lowtemperature combustion (LTC) strategy, especially as far as soot and NO<sub>x</sub> are concerned [5-8]. However, if properly optimized, the adoption of pilot injections in combination with low-temperature combustion strategies may help compensate for their drawbacks, including reducing overall HC and CO emissions that are among the major challenges of low-temperature combustion modes.

Computational modeling of pilot injection phenomena may aid experimental investigations by providing more insight into how mixture preparation develops and what are the sources of ignition and pollutant formation. As a matter of fact, the reliability of detailed engine computer models is crucial to the development and assessment of new combustion concepts for internal combustion engines, such as homogeneous-charge compression ignition (HCCI), partially-premixed combustion (PPC), and reactivity-controlled compression ignition (RCCI). However, typical computational model validations are carried out against simplified, reference benchmarks that are not always able to represent the full range of conditions at which models are requested to perform. This is particularly true when looking at light-duty diesel engines, where the fuel spray is injected in highly swirling environments, and typical injection strategies feature massive jet impingement and flow separation at the piston bowl rim. A number of previous studies have shown how engine computational fluid dynamics (CFD) models can be used effectively to capture mixture preparation and ignition in low-temperature, partially premixed combustion strategies, and aid in the understanding of the main sources of pollutant emissions arising from overly lean mixtures forming below the ignition limits. However, there is lack of validation studies considering the transient conditions typical of pilot injections, which feature small injected masses, low injection pressures and non-steady injector needle behavior. The aim of this study was thus to assess and validate a CFD engine model for simulating pilot injection phenomena in the Sandia light-duty optical diesel engine, operated with a Diesel Primary Reference Fuel mixture. Extensive experimental campaigns have been conducted on this engine to measure and understand the mixture preparation and pilot ignition limits for a wide range of operating conditions relevant to low-temperature combustion strategies [9,10].

The study is structured as follows. First, the major details of the experimental campaigns are given. Then, the computational methodology is described, and the sub-models chosen to describe the spray physical processes and the ignition kinetics are studied for some simple, fundamental test-cases. Finally, the model's reliability with varying operating parameters is assessed against local equivalence ratio measurements of [9], and the ignitability limits of a pilot injection over a range of charge dilutions and pilot injection parameters are modeled and compared to the experiments of [10].

# **Experimental setup**

All of the experimental measurements were carried out using the Sandia National Laboratories light-duty optical engine facility [9,10]. The engine used in the studies is a modified version of the GM light-duty 1.9L engine, provided with an optical piston that retains the full geometric details of the production piston. Optical access to the combustion chamber allows extensive measurements of local quantities in the squish region and in the piston bowl, as schematically represented in Figure 1. The engine is also provided with a variable swirl generation device placed upstream of the intake valves, which features adjustable throttle plates. Different throttling strategies can be used to generate swirl ratios from about 1.5 up to about 5.5. A summary of the main engine characteristics, along with the injector parameters and composition of the fuel used in the experiments, is reported in Table 1.

All of the pilot injection experiments considered in this study were run at a fixed engine speed of 1500 rev/min, and with variable intake conditions, but keeping an approximately constant average near-TDC ambient density of 19.6 kg/m<sup>3</sup>. The timing of the single pilot injection was held fixed at 15° before top dead center (TDC), so as to limit the impact of spray targeting, variable in-cylinder flows, and transients in the in-cylinder density and temperature on the ignition and mixture formation process. The primary independent variables were thus near-TDC temperature, ambient  $O_2$  concentration, pilot mass, injection pressure, and swirl ratio.

Although ignition studies were carried out in environments with different  $O_2$  concentrations, measurements of the mixture formation process (local equivalence ratio distributions) were taken in a non-reacting environment of pure nitrogen using a fuel tracer-based planar laser-induced fluorescence technique (PLIF).



Figure 1 - Schematic representing the optical access engine setup, including the three laser sheet locations and camera viewing direction (from [9]).

Table 1 - Main engine and experimental setup specifications for the experimental pilot injection campaigns.

#### **Engine specifications**

Bore x stroke [mm]	82.0 x 90.4
Unit displacement [cm <sup>3</sup> ]	477.2
Compression ratio	16.4 : 1
Squish height at TDC [mm]	0.88

#### **Bosch CRI2.2 Injector parameters**

Sac volume [mm <sup>3</sup> ]	0.23
Number of holes	7
Included angle [deg]	149
Nozzle diameter [mm]	0.14
Hole protrusion [mm]	0.3

### Fuel properties for PLIF studies

Composition [mole fractions]	$42\% nC_{16}H_{34}$
	58% iso-C <sub>16</sub> H <sub>34</sub>
Fluorescent tracer [mass fraction]	0.5% 1-C <sub>11</sub> H <sub>10</sub>
Equivalent Cetane Number [-]	50.7

### Fuel properties for ignition studies

US #2 diesel fuel	CN=47

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Table 2 - Operating conditions details for both the reacting (ignition
studies) and non-reacting (mixture formation studies) cases.

Non-reacting intake charge composition [mole fractions]	100% N <sub>2</sub>
Non-reacting intake temperatures [K]	300, 381
Reacting intake charge composition [mole fractions]	10% O <sub>2</sub> ,81% N <sub>2</sub> ,9% CO <sub>2</sub> 12% O <sub>2</sub> ,80% N <sub>2</sub> ,8% CO <sub>2</sub> 14% O <sub>2</sub> ,80% N <sub>2</sub> ,6% CO <sub>2</sub> 16% O <sub>2</sub> ,80% N <sub>2</sub> ,4% CO <sub>2</sub> 18% O <sub>2</sub> ,79% N <sub>2</sub> ,3% CO <sub>2</sub>
Intake temperatures [K]	303, 323, 363, 403
Engine speed [rpm]	1500
Injected fuel mass [mg]	1.0, 2.0, 3.0, 4.0
Start of Injection [deg]	$-15.0 \pm 0.1$

An absence of  $O_2$  was required to avoid excessive fluorescence quenching of the 1-methylnaphtalene tracer that was added to the diesel primary reference fuel (DPRF) mixture. Use of the DPRF fuels was required to minimize fluorescence from species other than the 1methylnaphtalene. Two different intake temperatures were employed to investigate the impact of temperature on the mixture formation process. The PLIF measurements were made in three moving planes to track the mixture preparation process, as reported in Figure 2. One plane bisected the squish region, one was located at the bowl rim height and one was deeper within the piston bowl, at its maximum radius.

Experiments with ignitable intake charges were made for a matrix of charge compositions, corresponding to in-cylinder oxygen concentrations from 18% down to 10%, as well as near-TDC temperatures ranging from approximately 800K up to more than 950K. A summary of the experimental conditions for both the non-reacting and the reacting cases is reported in Table 2.

Finally, as noted above, a DPRF mixture was used for the PLIF imaging. The blend featured two cetane isomers, 42% n-hexadecane and 58% 2,2,4,4,6,8,8-heptamethylnonane (or iso-cetane) by volume. These proportions were selected to mimic well the ignition properties of the US #2 diesel fuel used in the ignitability experiments, with a cetane number of CN = 47 measured using ASTM D613. Note that the fuel mixture has a higher cetane number, CN = 50.7, than the #2 diesel fuel – despite the well-matched ignition behavior. The DPRF58 surrogate more closely matches the representative physical properties of the diesel fuel than a previously used, lighter and significantly more volatile PRF25 mixture [11,12], made up of 25% iso-octane and 75% n-heptane by volume, that had similar ignition characteristics as diesel fuel [39] but different physical properties relevant to spray injection, atomization and vaporization.

# Model development

The experimental campaigns of [9,10] provide a unique opportunity for the validation of spray models for internal combustion engine simulations, since the exact fuel components can be modeled for the physical processes occurring in the engine: injection, atomization, vaporization, and mixing and ignition. Although the ignitability studies were conducted with the #2 diesel fuel, the careful matching of the ignition behavior tothe DPRF blend, and to the PRF25 blends used in earlier work [11,12] allows the chemical modeling to be pursued with confidence.

Furthermore, modeling of pilot injection phenomena is a challenging task for computational modeling as the fuel injection process is fully transient and the injector needle never reaches its maximum lift (cf. Figure 16). This also affects the experimental campaigns, where the effects of stochastic phenomena are amplified, including interferences due to presence of residual liquid-phase fuel, or non-consistent nozzle-by-nozzle behavior due to internal injector dynamics and surface in-homogeneities [9]. For these reasons, in order to define an accurate computational model setup for the engine simulations, the choice of appropriate sub-models was based on validations against more fundamental test cases.

### Numerical setup and improvements to KIVA

The study was carried out using a modified version of the KIVA-ERC code, a custom build of the KIVA3V CFD code [13] that features improved sub-models for fuel spray, turbulence, heat transfer and combustion modeling. Fast, detailed chemical kinetics capability was added to the code by using the SpeedCHEM sparse analytical Jacobian chemistry solver [14], and a High-Dimensional Clustering (HDC) algorithm [15,16,40] for chemistry cell grouping. Furthermore, a piston compressibility model, previously developed and validated for the current engine facility, was used. This model noticeably improved the prediction of the cylinder compression ratio without needing to artificially modify the in-cylinder volume to match the measured pressure trace[17]. Details of the commonly used turbulence, spray and heat transfer sub-models activated for the present study are reported in Table 3.



Figure 2.View of the measurement planes on a vertical crosssectional cut-plane of the combustion chamber sector geometry.



Figure 3 - View of the computational grid used for this study near TDC.

Previous studies [17,18] have pointed out the need for using an appropriate grid resolution in order to correctly capture fuel vapor penetration for low-load, partially premixed compression ignition cases. This led to a converged grid resolution slightly smaller than 1 mm, with about 105k cells at bottom dead center (BDC),as represented in Figure 3. As the original KIVA3 code structure was not developed for such large domains, the simulations were extremely inefficient, leading to large computational times even for simple, motoring or non-reacting operating conditions. Thus, significant modifications in the code's architecture were introduced to make it more suitable for extensive computations with refined geometries, while maintaining the underlying numerical algorithms. The major modifications can be divided into three major classes:

- Removal of all static common-block structures and their replacement with modern, fully encapsulated and dynamically allocated Fortran modules;
- 2. Refactoring of the code's time-step restart capability, with selective storage/retrieval of the relevant simulation parameters based on the instantaneous simulation status (presence of spray drop parcels, activation of select sub-models, etc.);
- 3. Replacement of computationally expensive temperaturedependent functions, including thermo-chemistry and physical property functions of the gas-phase and liquid mixtures with SpeedCHEM's optimal-degree interpolation approach [14].

The updated code was found to provide identical results as the previous build, while achieving noticeable computational speed-ups for both small and large grids. As an example, a comparison between the previous and the current release of the code in terms of fluid flow solver CPU times is reported in Figure 4. Here, two extreme cases are compared: motored engine operation with a refined 2D mesh having only about 3000 cells at BDC and the same resolution as the mesh used in this study, and non-reacting pilot injection simulation using the grid with about 105000 cells at BDC of Figure 3. For the simple 2D simulation, requested CPU time was reduced by about 3.2 times to less than two minutes on a single core, while for the sector mesh setup relevant to this study the computational time was reduced from 29.9 hours down to less than 13 hours, corresponding to an overall speed-up by a factor of about 2.3.

Table 3 - Main sub-models activated in the KIVA-ERC+ code for
modeling pilot injections in the Sandia-GM optical engine.

Phenomenon	Sub-model
Spray breakup	KH-RT instability, Beale and Reitz [19]
Near-nozzle flow	Gas-jet theory, Abani et al. [20]
Spray angle	Reitz and Bracco [21]
Droplet collision	O'Rourke model [22] with ROI (radius-of- influence), [20]
Wall film	O'Rourke and Amsden [22]
Evaporation	Discrete multi-component, Ra and Reitz [23]
Turbulence	RNG k- ε, Han and Reitz [24]
Combustion	SpeedCHEM, Perini et al. [14,16]
Chemistry grouping	High-Dimensional Clustering, Perini et al. [15,16, 40], with $\varepsilon_T = 10 \text{ K}, \varepsilon_Y = 10^{-4}$
Optical piston compressibility	Perini et al. [17]

Diesel Primary Reference Fuel modeling

As described earlier, the present 42%/58% mass distribution of the DPRF58 surrogate was found in the experiments to yield the same ignition timings as a US #2 Diesel fuel [11,12]. Since the overall ignition event is the result of a chain of physical and chemical processes involving fuel spray atomization and evaporation, mixture formation and charge ignition kinetics, it was chosen to model the fuel liquid and gas phases in the engine model as



Figure 4 - CPU time comparison between the standard and current build of KIVA-ERC. (left) 2D motored case, (right) 3D sector non-reacting pilot injection case.

close as possible to the real fuel used in the experiments, in terms of both physical and thermo-chemical properties. Thus, liquid and gasphase fuel component properties were obtained from the pure hydrocarbons' database of Daubert and Danner [25], while the JANAF thermo-chemistry cards in the reaction mechanism for Diesel Primary Reference Fuels by Westbrook et al. [26] were used for gasphase modeling. It should be noted that, even if the ideal gas formulation in KIVA was used, at the operating conditions tested in this study, a real-gas equation of state could have anon-negligible effect on predicted local charge vaporization cooling.

Unlike the modeling of the physical spray dynamics and vaporization processes, it was not possible to model the ignition processes using only exact multi-component models for the diesel primary reference fuel used in the experiments, due to the fact that a sufficiently reduced chemical kinetics model for ignition of DPRF surrogates is not available. The detailed model by Westbrook et al. [26] features 2837 species and 10719 reactions, and, even with sparse chemistry capabilities, its incorporation was made impossible by the excessive computational burden required to advect this huge number of species.

Thus, the widely used approach that separates the physical spray behavior from the ignition kinetics was adopted. Since the ignition of the PRF25 of [17,18] was found to be similar to the DPRF58 fuel of the current study, the ERC PRF reaction mechanism was used [27]. The spray modeling used the physical properties of DPRF58.

### Fuel property determination

Mixture-averaged physical properties for DPRF58 were determined and single-component-equivalent fitting coefficients were computed over the temperature range of the liquid phase and introduced in the fuel library. The coefficients and the formulations used are reported in Appendix A.

The predictive capabilities of the model were assessed for three test cases: adiabatic evaporative cooling of liquid fuel; vaporization of a single droplet in a steady environment; ignition of a PRF or DPRF mixture in a homogeneous, constant-volume adiabatic reactor.

#### Mixture evaporative cooling

In order to test if the local temperature of a DPRF mixture after vaporization would be appropriate for modeling with PRF25 reaction kinetics, a mixture evaporative cooling test case was developed and its equivalence ratio sensitivity was studied. In order to find the final mixture properties, the program computes the final mixture thermal properties through three discrete states:

 $T_L$ 

 $T_L$ 

 A) Initial state: Liquid fuel (f) at temperature Gas-phase air (a) at temperature T<sub>A</sub>
B) Vaporized state:

Vaporized state: Fuel vapor (f) at temperature Gas-phase air (a) at temperature  $T_B$ where:

$$f(T_{B}) = \frac{A}{F} (h_{a}(T_{A}) - h_{a}(T_{B})) - h_{f,lv}(T_{L}) = 0;$$



Figure 5 - Evaporative cooling effects of PRF25 and DPRF58 fuels: amount of cooling after fuel vaporization and mixing versus the initial charge temperature, at a liquid fuel temperature  $T_{fuel} = 360$  K, and different final mixture equivalence ratios.

C) Fully mixed state:

Gas-phase air+fuel mixture (m) at temperature  $T_M$  where:

$$\mathbf{Y}_{m} = \left[\frac{A}{F}\mathbf{Y}_{a} + \mathbf{Y}_{f}\right] / \left[\frac{A}{F} + 1\right],$$
  
$$f(T_{M}) = \left(\frac{A}{F}h_{a}(T_{B}) + h_{f}(T_{L})\right) - h_{m}(T_{M}) = 0.$$

As shown in Figure 5 for an initial liquid fuel temperature of 360K and different initial charge temperatures close to the near-TDC conditions tested in the current study, PRF25 and DPRF58 have similar cooling effects. The same analysis carried out for different PRF numbers and DPRF numbers, as reported in Figure 6, did not show noticeable changes in these results, confirming that, provided the final equivalence ratio is the same, both fuel representations lead to similar adiabatic mixture temperatures, thus leaving ignition timing to rely on the suitability of the kinetics modeling.

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#### Droplet vaporization process

Both atomization and vaporization have a crucial effect on the predicted spray structure and mixture preparation. It was found that calibration of the Kelvin-Helmholtz Rayleigh-Taylor (KH-RT) model constants had little effect on predicted liquid fuel penetration and gasphase mixture preparation when simulating short, pilot injections. The KH time scale constant  $B_I$  of [19] was varied from  $B_I = 10$  to 80, and the previously established value of  $B_I = 40$  [17] was eventually chosen. To validate and to examine the impact of the fuel vaporization modeling, in this section the vaporization behavior of the discrete multi-component fuel model used was assessed for both single- and multi-component fuel compositions.

The evaporation of a single n-heptane droplet in a steady environment under micro-gravity conditions was modeled and validated against the experiments by Nomura et al. [28] – see Figure 7.



Figure 6 - Evaporative cooling effects of DPRF number liquid fuels at different final equivalence ratio. Liquid fuel temperature  $T_{fuel} = 360K$ , initial charge temperature  $T_{air} = 800K$ .

The simulation matched the experiment; however, the initial liquid drop temperature was not known, and was assumed to be T = 330 K. The initial and transient droplet temperature behavior is a primary source of uncertainty in single droplet evaporation experiments, where the droplet itself is suspended from one or more threads, and thermal conductivity effects cannot be avoided [28]. However, the model showed good agreement with the measured vaporization histories.

The same setup was used to compare the vaporization histories of the DPRF58 mixture, when modeled 1) as a single component with the mixture-averaged physical properties described earlier, or 2) as a binary liquid mixture. In Figure 8, the vaporization history using the two approaches is compared in a high-pressure environment and at temperatures relevant to near-TDC engine conditions, with an initial drop diameter d = 0.7 mm and temperature T = 330K. In either case, the model clearly captures the initial thermal expansion effects due to heating of the droplet in the high-temperature environment. As far as the vaporization diameter slope is concerned, the single-component model cannot represent the different volatilities of the two fuel components, and the mixture-averaged behavior leads to a slightly faster vaporization at low temperatures. However, the difference

between the two approaches narrows as temperature increases and the overall vaporization process is very well captured at high temperatures. It is expected that these differences become negligible in the engine, where the vaporization process is ruled by significant convective heat transfer. Thus, the single-component approach is an effective way to model the vaporization of the DPRF mixture, the ignition of which is modeled using PRF kinetics.



Figure 7 - Predicted (DMC model of Ra and Reitz [23]) vs. measured (Nomura 1996, [28]) vaporization histories of a single n-heptane droplet in a steady high-temperature environment under microgravity conditions.



Figure 8 - Predicted vaporization history of a single DPRF58 droplet, with initial radius of 0.7 mm, in a steady, high-temperature and high-pressure environment. (solid lines) single-component averaged fuel properties; (dashed lines) full multi-component model.

Finally, single drop vaporization was used to compare predicted vaporization histories of the two fuel surrogates using the multicomponent model. In Figure 9 the predicted PRF25 vaporization was completed between 2.66 times and 3.86 times faster than the DPRF58 droplet, due to its one order of magnitude higher vapor pressure. These results suggest that similar overall ignition timings in the Page 6 of 15 engine could be seen when PRF25 and DPRF58 fuel blends are compared. With PRF25, the shorter vaporization time (related to the physical component of ignition delay) will, at moderate temperatures and slightly rich equivalence ratios, be compensated for by a longer chemical ignition delay – as shown in a subsequent section.



Figure 9 - Vaporization histories of single droplets of either DPRF58 (solid lines) or PRF25 (dashed lines) composition in a steady, high-temperature and high-pressure environment.

#### Gas-phase kinetics modeling

Ignition of PRF25 was modeled using the skeletal mechanism for Primary Reference Fuels (ERC-PRF) by Ra and Reitz, featuring 47 species and 142 reactions [27]. Of the two versions published in [27], the more reactive version was used. This version provides better ignition delay predictions for slightly rich mixtures, suitable for the rich mixture pockets that drive ignition in spray-induced combustion, and was also validated against compression ignition internal combustion engine simulations. In particular, this mechanism was shown to match experimental ignition delay times of shock tube data with rich mixtures. As represented in Figure 10, the mechanism has been found to also capture well ignition delay timings of even stoichiometric and lean mixtures in shock tubes, when in the high pressure range relevant to the present study.

The choice of using a PRF25 mixture as representative ignition kinetics for the DPRF58 diesel surrogate mixture used in this study was driven by the observation, in a previous study, that both these diesel surrogates provided very similar ignition timings and heat release rate trends (HRR) to a CN 47 US diesel fuel, when operating the engine in this study with a partially-premixed combustion strategy [39].



Figure 10 - Predicted ignition delays for lean and stoichiometric nheptane/air mixture at elevated pressures, using the ERC PRF mechanism [27]. Comparison with experimental measurements of [29-33].

Thus, further investigation of the impact of utilizing PRF25 kinetics in the engine simulation, predicted ignition delays of PRF mixtures in a constant-volume vessel were compared with predicted DPRF58 ignition delays using the detailed mechanism of Westbrook et al. [26] at three representative mixture equivalence ratios. The calculations were run with the SpeedCHEM-ignition delay module [14]. The results are summarized in Figure 11.



Figure 11 - Ignition delay comparison for different fuel/air mixtures at elevated pressure and equivalence ratios of 0.5, 1.0, 2.0: DPRF58 kinetics [26] versus PRF kinetics [27] at PRF0, PRF25, PRF50, PRF100 compositions.

The NTC region for DPRF58 is less pronounced than for the PRF mixtures in the low PRF number range. DPRF58 ignition delays are similar to fuels with high PRF numbers (PRF > 50) at the lowest temperatures (i.e., T < 750 K), and low PRF fuels at high temperatures (i.e., T > 1000K). The intermediate temperature range, i.e., 750 K < T < 1000 K, is relevant to the near-TDC conditions in the light-duty engine where ignition of the pilot injection occurs [10].

Here, DPRF58 shows a plateau with roughly constant ignition delays and very little temperature sensitivity.

The equivalence ratio sensitivity of DPRF58 is much higher than for the PRFs, especially in the intermediate temperature range. Here, the ignition delay spans from about 500  $\mu$ s for a moderately rich  $\phi = 2.0$ mixture up to about 2500  $\mu$ s for a lean  $\phi = 0.5$  mixture. From the plots it is also evident that when ignition falls in this intermediate temperature region, and at moderately rich mixtures, PRF25 appears to be a good surrogate with similar ignition kinetics as DPRF58.

Finally, using PRF25 is suitable also for the high temperature range, where the PRF and DPRF fuels show similar ignition delays. It should be noted, however, that there is a window of temperatures for very rich mixtures and intermediate temperatures (900 K < T < 1000 K) where no PRF composition is able to capture the faster ignition kinetics of the diesel primary reference fuel. This may not have a significant impact for small injected mass values, but may affect pilot ignition for the largest mass values, where significant fuel rich regions were observed [9]. Thus, there is a need to develop a reduced chemical kinetic model for DPRF ignition in order to properly capture the fuel's kinetics.

# In-cylinder flow modeling

Previous studies showed the significant impact of local flow field quantities on the mixture distribution fields created by main and pilot injections in the SNL light-duty optical engine facility [9-12]. In order to match near-TDC swirl flow velocities, full engine geometry simulations were used to predict in-cylinder fluid flow quantities and provide initialization parameters for the sector mesh simulations used in the present study.



Figure 12–Details of the full engine geometry used for the intake stroke calculations.



Figure 13 - Sample throttle orientations for modeling the actual swirl generation by intake port throttling strategies with the full engine geometry.

Table 4- Experimental [35] and calculated [34] swirl ratios for the four swirl conditions used in this study, and corresponding helical (H) and tangential (T) pin positions in the experiments.

Rs, Swirl meter	Rs @IVC, full mesh	Н	Т
1.50	1.393	15	7
2.20	2.091	19	19
3.50	3.895	7	19
4.50	4.804	5	19

A computational grid with 559867 cells and 585189 vertices at BDC was used, as represented in Figure 12. The accuracy of the fluid flow predictions was assessed in [34], and good agreement of the model's predictions with 1) local near-TDC tangential velocity profiles; 2) swirl center precession and tilting behavior was found.



Figure 14 - Predicted velocity field magnitude structures at BDC during the induction stroke using the full engine geometry model. (from left to right) Rs = 1.5, 2.2, 3.5, 4.5. (top) top view, (bottom) vertical cross-section at the intake ports.



Figure 15 - Comparison between predicted in-cylinder swirl ratios using full mesh and induction stroke calculations and IVC-initialized sector mesh simulations.

Different swirl ratios are obtained in the engine by throttling the intake ports [36]. Two throttle valves are placed immediately upstream of the intake valves, and swirl ratios ranging from  $R_s = 1.5$  up to  $R_s = 4.5$  are achieved by throttling either the tangential or the helical port, according to the strategy reported in Table 4. Discrete pin positions allow throttle orientations from a fully closed (pin = 0) to a wide open position (pin = 19). The throttle was introduced in the engine model through a mesh modification algorithm that deactivates grid cells in the region near the throttle, and sets their face boundary types as solid walls and finally rotates the plate at the desired angle. In Figure 13 some of the throttle orientations are illustrated. Full details of the variable throttling model are reported in [34].

In Ref. [34] it was also found that the nominal swirl ratios measured on the swirl bench were not representative of the instantaneous swirl conditions at IVC, where the sector simulations are typically initialized, and thus were not used as initialization parameters for the simulations in this study. As reported in Figure 14, where a top view of the cylinder and a vertical cross section of the velocity magnitude field at the intake valves are reported, the velocity flow field in the full engine geometry is far from being axisymmetric, and the overall swirl ratio value around the cylinder axis is not well representative of the instantaneous swirling momentum. Furthermore, the simplified, axisymmetric geometric representation of the piston surface and of the cylinder head in the sector mesh quickly dampens the amount of in-homogeneity into a fully axisymmetric flow field even after just a few solver time-steps. This is shown in Figure 15. While in the full engine model the non-homogeneity of the swirling flow leads to its progressive dissipation up to about 45 degrees before top dead center, in the sector mesh the smooth swirl vortex structure leads to much stronger momentum conservation, so that the instantaneous swirl ratio significantly increases even from the early stages of the compression stroke.

For these reasons, the IVC swirl conditions must be lowered in order to match the effective swirl ratios predicted with the full engine geometry at TDC. The required swirl ratios at the initialization to match the near-TDC swirl ratios of the full mesh simulation were Rs = 1.236, 1.856, 3.502, 4.303.

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# **Results**

#### Equivalence Ratio predictions

The model was validated against local equivalence ratio measurements by Sahoo et al. [9]. The experiments featured wide ranges of operating conditions, including injected mass of 1 up to 4 mg, intake temperatures leading to near-TDC temperatures from about 815 K up to about 960 K, swirl ratios of  $R_s = 2.2$  and 4.5, and injection pressures of 500 bar and 860 bar. Injection profiles were modeled by extrapolation from measured injection rates[17], as seen in Figure 16.

For the model validation, the operating conditions featured 4 mg injected fuel mass, baseline swirl ratio  $R_s = 2.2$ , 930 K ambient temperature and injection pressure of 500 and 860 bar. In Figure 17, predictions of local equivalence ratios for an injected mass of 4 mg, injection pressure of 860 bar, and a near-TDC temperature of 930K are compared with the corresponding PLIF images.



Figure 16 - Pilot injection mass flow rates used for the simulations, obtained from experimentally measured rates with the Bosch CRIP2.2 injector at an injected mass m = 8.8 mg.

In the experiments, the three fuel jets, at the top-left, top-right and bottom-right, as reported in Figures from 17 to 20, exhibited systematically distinct behavior from all the other jets and were thus not considered for the comparison.

The simulations showed good agreement with the measurements on plane P1: signs of jet impingement against the rim already appear at 10 degrees before TDC, and lean fuel-air mixtures are seen in the jet core up to TDC in the jet region that does not impact against the rim. The equivalence ratios become overly lean as the piston approaches TDC. Also the fuel rebound after impacting against the rim was properly captured, but to a smaller extent than seen in the experiment. By examining a vertical cross-section of the combustion chamber, it was seen that most of the fuel impacting against the bowl rim was directed downwards into the bowl instead of upwards. This may be caused by a larger-than-predicted spray angle or by an inaccurately captured spray jet orientation. Interestingly, while the injector has a nominal spray cone angle of 12.0 degrees, the dynamic spray angle model by Reitz and Bracco [21] yielded actual spray angles between 14.0 and 15.5 degrees at 860 bar injection pressure and at the present

combustion chamber conditions. This seems to be more consistent with the experiments, where no coherent conical spray jet structure can be seen, but where all the spray jets show significant thickness even extremely close to the nozzle. Finally, both penetration and equivalence ratios are reasonably well-captured at the bowl rim plane, although the simulations show a slight lack of mixing evidenced by the breadth of the fuel jets (especially at the earlier crank angles), and a smaller fuel amount tends to be found near the bowl rim plane. The experimental measurements also show a tendency towards formation of higher peak equivalence ratios near the impact region.

As injection pressure is reduced to 500 bar in Figure 18, the model is seen to behave consistently with the changes in jet penetration seen in the experiment. Smaller penetration is predicted and, consistent with the experiment, the first signs of fuel being redirected after impingement against the rim appear between 6 and 4 degrees bTDC. Here, the simulation shows the most accurate results at the earliest crank angles. However, there is a tendency towards predicting smaller equivalence ratios than measured as the piston moves towards top dead center. The reduction in jet penetration brought by the lower injection pressure also leads to higher equivalence ratios than at 860 bar. Again, non-negligible jet-to-jet variations are seen in the experiments that cannot be predicted by the model.

Simulation results with different injected masses are compared to the experiments in Figure 20, halfway between the start of injection and TDC. Good agreement of the simulation with the experiments is seen, and larger injected mass leads to increased penetration and richer equivalence ratios. The modeling appears to have properly captured the jet dynamics even at the smallest 1 mg injected mass, where the spray jets have not impacted against the rim, but a significant portion of the jet tip has already penetrated into that region. Consistent with the experiments, increased injected fuel mass also leads to greater penetration, leading to greater concentrations at the rim plane and in the squish region.

The effects of ambient temperature on the predicted spray jet properties are reported in Figure 19 for near-TDC temperatures of 850 K and 930 K, and injected mass of 2 mg. The reduced temperature makes the vaporization process longer and thus increases the liquid phase lifetime, increasing liquid penetration. The effect seen is that, before impacting against the rim, slightly smaller vapor equivalence ratios are seen for the higher temperature case. The experimental measurements appear to show instead a slight increase in equivalence ratios.



Figure 17 - Model validation against measured fuel distributions. Ambient temperature = 930 K, injected mass = 4 mg, Rs = 2.2, injection pressure of 860 bar; planes P1 (top two rows) and P2 (bottom two rows). Upper row: KIVA, lower row: experiment [9].

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Figure 18 - Model validation against measured fuel distributions. Ambient temperature = 930 K, injected mass = 4 mg, Rs = 2.2, injection pressure of 500 bar; planes P1 (top two rows) and P2 (bottom two rows). Upper row: KIVA, lower row: experiment [9].



Figure 19 - Ambient temperature effects on predicted fuel distribution. Near-TDC temperature 850 K (left) and 930 K (right). Injected mass = 2 mg, Rs = 2.2, injection pressure 860 bar;.

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Figure 20 - Injected mass sweep at  $p_{inj} = 860$  bar, Rs = 2.2, 930K, 8 deg bTDC. KIVA simulations versus experiments.

### Ignitability of a pilot injection

Once the overall spray modeling had been validated against the local equivalence ratio measurements of [9], fired engine simulations were run for the conditions of the experimental study in [10].

As not enough heat release is present when a pilot injection ignites to sharply affect the measured pressure trace, we used the "robust" ignition criterion of Miles et al. [10], where ignition is defined to have happened when energy corresponding to at least 40% of the lower heating value of the fuel has been released before 10 degrees after TDC (when a hypothetical main injection is supposed to start). A matrix of 20 calculations was run for every injected fuel amount and injection pressure condition, matching the charge dilution and near-TDC temperatures used in the experiments, as summarized in Table 2. In Figure 21, predicted ignitability temperatures are compared with the corresponding experimentally measured thresholds. The predicted near-TDC temperatures, the simulations do show some discrepancies:

- The injected-mass dependency of the ignitability temperature is larger than seen in the experiments, i.e., predicted ignitability temperatures for the smallest injected masses are higher than measured, this being relevant especially for the 1 mg cases;
- 2) At 500 bar, the predicted ignitability temperature is overestimated by approximately 20 to 50 K even at the largest injected fuel amounts;
- 3) At 860 bar, similar ignitability threshold values to the experiments are seen for injected masses of 2 and 3 mg, but with a slightly steeper behavior, leading to increased ignitability limits at the lower oxygen concentrations.



Figure 21 - Computed (marks) and experimental (lines) variation of pilot ignition temperature versus oxygen concentration for various pilot injection mass and pressure values. Dots represent the matrix of operating conditions tested.

The overall model behavior is however consistent with the experiments in terms of the predicted ignitability trends, and also the threshold values appear to be reasonably well captured at the highest injection pressure and largest injected mass conditions.

# Conclusions

A comprehensive sector mesh model for the simulation of the ignitability of pilot injections in the Sandia light-duty optical diesel engine facility using a DPRF58 diesel primary reference fuel was validated. An extensive set of planar laser-induced fluorescence (PLIF) experiments was used to validate the spray predictions in terms of fuel jet penetration and mixture formation at different pilot-injected mass, injection pressure, ambient temperature and swirl ratio values. Finally, the pilot ignitability characteristics in dilute environments, spanning charge oxygen concentrations from 10% to 18% were studied.

The following conclusions were drawn:

- Small differences were observed in the vaporization behavior when considering the fuel as a single component, with mixtureaveraged properties, or as a binary component;
- Detailed engine modeling accurately captured the intake swirl conditions; this allowed resolution of swirl effects on the fuel jet

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distortion. Further improvements in flow field predictions may be achieved by introducing the full geometry representation of the combustion chamber and intake/exhaust ducts, as the axisymmetric assumption was seen to quickly dampen nonhomogeneities after initialization;

- The skeletal PRF mechanism matched ignition behavior occurring in the temperature range (900-1100 K) of interest for evaluating the ignitability of a pilot injection. In comparison, the detailed DPRF mechanism showed differences in the DPRF58 ignition behavior in the negative temperature coefficient (NTC) temperature region, with DPRF58 achieving significantly faster ignition for rich mixtures.
- The simulated pilot injection ignitabilities were consistent with the experiments, but were shifted to higher temperatures and oxygen concentrations. Faster DPRF58 kinetics, and jet-by-jet variabilities, not currently predicted by the model may have an effect on this phenomenon.

These conclusions also point out the need for future studies to focus on:

- More comprehensive modeling of the in-cylinder local thermal and flow field quantities, through usage of the full engine geometry representation and full induction stroke simulations;
- A fully coupled representation of the fuel's physical and chemical characteristics through the adoption/development of a reduced chemical kinetic scheme for the ignition of mixtures of n-hexadecane and heptamethylnonane for Diesel Primary Reference Fuel modeling.

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# Appendix A – DPRF58 fuel properties

The single-component-equivalent fuel properties for the DPRF58 binary mixture were determined starting from the single-component laws in Daubert and Danner [25]. The average mixture properties were evaluating using proper mass-based or mole-based averaging, and fitting coefficients suitable for the same law formulations were determined by solving a least-square problem at the same temperature range of validity of the singlecomponent formulations, or in the interval between  $T_0 = 298.15$  K and  $T_{crit} = 704.90$  K. The valid temperature interval for each property was subdivided into 1000 equally-spaced temperature points, and fitting coefficients were solved for through the Nelder-Mead simplex method [38].

Details of the liquid-phase mixture properties and their coefficients are reported in Table A1. The corresponding laws describing their behavior, as determined in [25], are also reported here for the sake of completeness:

$$f_1(T) = \frac{a}{h^{\left(1 + \left(1 - \frac{T}{c}\right)^d\right)}},$$
 (A1)  $f_2(T) = a(1 - T^*)^b, T^* = T/T_{crit},$  (A2)

(A5)

$$f_3(T) = \exp\left(a + \frac{b}{T} + c\log(T) + dT^e\right), \quad (A3)$$
$$f_5(T) = \left(aT^b\right) / \left(1 + \frac{c}{T} + \frac{d}{T^2}\right), \quad (A5)$$

$$f_4(T) = a + bT + cT^2 + dT^3 + eT^4$$
, (A4)

$$f_6(T) = \left(aT^b\right) / \left(1 + \frac{c}{T} + \frac{d}{T^2}\right). \tag{A6}$$

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property	formula	a	b	с	d	e
Critical temperature [K]			704	.90		
Molecular weight [g/mol]			226	.446		
Density [kmol/m <sup>3</sup> ]	A1	2.503e-1	2.448e-1	7.049e+2	2.742e-1	-
Heat of vaporization [J/kmol]	A2	1.767e+3	4.550e-1	-	-	-
Vapor pressure [Pa]	A3	1.400e+2	-1.414e4	-1.642e1	3.990e-6	2.000e0
Viscosity [Pa s]	A3	-3.060e1	2.691e3	2.779e0	0.000	0.000
Surface tension [N/m]	A2	5.154e-2	1.286e0	-	-	-
Heat capacity (constant pressure) [J/kg/K]	A4	3.091e+5	2.343e+2	1.124e0	0.000	0.000

Table A1. Fitting coefficients for the calculation of the physical properties of a liquid DPRF58 mixture

Finally, as far as gas-phase properties are concerned, the same approach was used to determine mixture-averaged properties for thermal conductivity, single-component viscosity and constant pressure heat capacity, as summarized in Table A2. A JANAF thermodynamic card for enthalpy, energy and entropy evaluations was instead determined based on the single-component properties in the detailed reaction mechanism by Westbrook et al. [26]. The card is reported in Figure A1.

property	Formula	a	b	с	d	e
Thermal conductivity[W/m/K]	A5	1.734e-5	1.281e0	5.577e2	-1.412e4	-
Viscosity[Pa s]	A5	1.727e-7	6.608e-1	2.340e2	6.488e1	-
Heat capacity (constant pressure) [J/kg/K]	A6	2.729e5	8.806e5	1.706e3	6.435e5	7.681e2

Table A2. Fitting coefficients for the calculation of the physical properties of a gas-phase DPRF58 mixture

HD42HMN58	sae2014 c 16 h 3	4 g	300.000 5000.000 1396.220	) 1
5.44758160e+01	7.10936084e-02-2.	41049317e-05	3.71054407e-09-2.10673139e-1	L3 2
-7.52250544e+04	-2.61411665e+02-7.	78659232e+00	2.18293284e-01-1.56950128e-0	)4 3
5.81608619e-08	-8.76080720e-12-5.	39014382e+04	7.21477969e+01	4

Figure A1. JANAF thermodynamic table for a gas-phase DPRF58 mixture