# Increased Particle Emissions from Early Fuel Injection Timing Diesel Low Temperature Combustion

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ABSTRACT

A clean premixed Diesel combustion strategy, called low temperature combustion (LTC), was able to achieve very low nitrogen oxide emissions (<35 ppm) through use of exhaust gas recirculation (12.1% Inlet Oxygen), and reduced particulate matter (PM) emissions (<0.05 FSN) through advanced fuel injection timing (-24°aTDC). When varying the injection timing by relatively small increments, large changes in PM mass and number emissions were measured within the premixed LTC regime. A discrepancy is investigated between predicted reductions in PM emissions by simple fuel-air premixing and combustion temperature metrics, and actual PM emissions measurements when advancing the fuel injection timing earlier than -24°aTDC. For these earlier injection timings, particle numbers were seen to increase in two distinct particle size modes, whereas only one particle size mode existed at the minimum PM emissions -24°aTDC injection timing. Additional parameters from a 1D free fuel spray model were used to suggest new information that could explain the cause of these unexpected increases in PM. Using 0D and 1D calculations, the engine-out particle size and number emissions are analyzed

to better understand their sensitivity to changes in the fuel injection timing within the early injection timing LTC regime.

*Particle; Emissions; Premixed; Low; Temperature; Combustion*

## 1. Introduction

Diesel engines offer an inherent advantage of reduced fuel consumption and $CO_2$ emissions over other types of internal combustion engines due to their higher thermal efficiency. For this reason the Diesel engine is a common powerplant option for transportation, especially in medium and heavy duty vehicles. The drawback of conventional Diesel engines is their traditionally higher emissions levels of particulate matter (PM) and oxides of nitrogen ($NO_x$). Many researchers [1-4] have shown evidence of a correlation of ambient particle levels with hospital admissions and mortality rates (strongest correlations with respiratory and cardiovascular system ailments). Other studies [5-11] have suggested the importance of the ultrafine portion (smaller than 100nm) of all ambient particles on health effects. Diesel engines have been shown to emit a great deal of their particles (especially in particle number) in the ultrafine size range [12-16]. Therefore understanding the particle emissions characteristics from conventional and modern Diesel engines is important to better understanding their effects on the environment and human health.

New emissions regulations are obliging engine manufacturers to reduce these emissions far below previous levels. In-cylinder formation of Diesel soot aggregate particles occur in regions of high local richness and temperature [17,18]. Enhancinging the fuel and air mixing process in-cylinder before the start of combustion (SOC) and reducing the adiabatic flame temperature by the use of exhaust gas recirculation (EGR) in the Low Temperature Combustion (LTC) regime with modern Diesel engines has helped to decrease engine-out particulate matter (PM) mass emissions [19-22].

Although these LTC combustion concepts have greatly reduced engine-out PM mass emissions in comparison with conventional Diesel combustion, more comprehensive particle emissions measurements have shown a simultaneous decrease in the particle sizes, increase in particle organic fraction (volatility), and (depending on the LTC engine operating condition) a possible increase in particle numbers [14,15]. A recent publication [16] has shown that there can exist an early and a late fuel injection timing within the Diesel LTC regime for a given engine load and speed where engine-out PM emissions are possible at (or below) the minimum detection limit of a common opacity-based PM mass concentration measurement instrument. It was also described that although the PM mass emissions had been greatly reduced relative to conventional Diesel combustion, important changes still occurred in particle size and number emissions within the LTC regime (especially for particles smaller than 50nm). In this previous publication, advancement of the fuel injection timing from the timing of maximum PM (-9°aTDC) emissions led to elongation of the ignition delay (time from start of injection to start of combustion) and decreases in emissions of particulate mass and number concentrations. Thermodynamic calculations indicated that further increases in the ignition delay were possible with continued advancement of the injection timing beyond the point where PM emissions were already below the opacity-based instrument's minimum detection limit, thus predicting a further reduction in particulate mass and number emissions. But emissions measurements showed otherwise, that both PM mass and number emissions increased with further injection timing advances beyond the injection timing of the opacity-based instrument's minimum detection limit (-24°aTDC). The particle size distribution results revealed that there were increases in two distinct modes of particles, one mode to either side of 50nm when the injection timing was advanced. Using a 1D free spray analysis model [23,24], this work investigates if fuel spray-piston surface interactions caused PM mass and number emissions increases for further advanced injection timings within the Diesel LTC regime, though ignition delay and adiabatic flame temperature towards the end of combustion (reasons for decreases in engine-out PM emissions) both increased with further advancements of fuel injection timing.

## 2. Material and Methods

### *2.1 Engine*

The characteristics of the Diesel research engine used in this study are described in TABLE 1. The engine hardware was selected so that it could effectively operate in either the conventional Diesel mixing-controlled, or Diesel premixed LTC operating regime throughout the entire engine load and speed map.

**TABLE 1. Engine Characteristics**

| | |
|---|---|
| Engine Type | Single Cylinder, Direct-Injection, Four-Stroke |
| Bore x Stroke [mm] | 123 x 152 |
| Displacement [liter] | 1.806 |
| Compression Ratio | 14.4:1 |
| Injector Nozzle | Mini-Sac, 7 x 0.190mm |
| Injector Included Angle [°] | 120 |

TABLE 2 illustrates the engine operating conditions selected for this study. The range of injection timings selected for this study, -24 to -33 °aTDC, was selected to study the sensitivity of increased PM mass and number emissions with injection timing advancements earlier than the early minimum PM injection timing (-24°aTDC). The earliest injection timing in the study was limited to -33°aTDC to maintain in-cylinder pressure rise rates less than 22 bar/CAD. An intake oxygen concentration of 12.1% proved to be low enough to reduce the maximum adiabatic flame temperature below 2200K, and the NOx emissions below 35ppm (1.09 g/kg_fuel). The intake temperature, intake pressure, and EGR rate were selected to achieve a LTC engine operating condition while being consistent with realistic pre-production heavy duty Diesel engine capabilities.

**TABLE 2. LTC Engine Operating Condition**

| | |
|---|---|
| Speed [RPM] | 1200 |
| IMEP [bar] | ~7 |
| Fuel Injected [mg/cycle] | 70 |
| Start of Injection [°aTDC] | -24 to -33 |

| | |
|---|---|
| Injection Pressure [bar] | 1450 |
| EGR [%_vol] | 50 |
| Intake Oxygen [%_vol] | 12.1 |
| Equivalence Ratio [-] | 0.83 |
| Intake Temperature [°C] | 45 |
| Intake Pressure [bar] | 1.35 |
| Exhaust Temperature [°C] | 366 |
| Exhaust Pressure [bar] | 1.45 |

IMEP = Indicated Mean Effective Pressure

EGR = Exhaust Gas Recirculation

A commercially available European Diesel fuel was used in this study with a cetane number of 53.5, sulful content of 8.9ppm, PAH content of 1.3%(m/m), and a T95 of 356°C. These specific fuel properties were analyzed due to their influence on combustion generated nanoparticle emissions [25-29].

*2.2. Emissions Instruments*

A Horiba MEXA 7100 was used to measure the exhaust gaseous components of carbon dioxide ($CO_2$), carbon monoxide (CO), hydrocarbons (HC), and oxides of nitrogen ($NO_x$). An AVL Smokemeter 415 (opacity-based measurement) was used to measure the exhaust PM mass concentration. In order to make measurements of the particle size distribution with a TSI Scanning Mobility Particle Sizer (SMPS), a dual-stage partial exhaust dilution was performed using a Dekati FPS-4000.

The exhaust sample temperature was measured to be 295°C in the engine exhaust system at the point where the exhaust sample was extracted by the dilution system. The dilution system inlet sample probe temperature was regulated as close as possible (but not exceeding) the exhaust sample temperature, at 290°C. The primary dilution heater setpoint temperature was set to the maximum recommended by the diluter manufacturer, 300°C. The actual temperature of the primary dilution air once it entered the diluter body, as measured by an internal thermocouple just before the point of mixing with the exhaust sample, was 182°C due to heat losses during transfer to the diluter body. Although the primary dilution was performed with 5.9lpm of heated dilution air, the 162lpm of secondary dilution air was at ambient temperature. The secondary dilution air flow was maximized for this diluter and the primary dilution air flow was adjusted to achieve the overall 40:1 total dilution ratio.

The TSI SMPS 3936 consisted of the TSI 3080L electrostatic classifier with a long Differential Mobility Analyzer (DMA) and a TSI 3010 Condensation Particle Counter (CPC). Particle concentration units of the size distribution are displayed in dN/dlogDp (particle number per cubic centimeter), meaning that the particle number concentration has been weighted by particle number (the instrument's base unit) and normalized to one decade of particle size so that particle size distributions from various instruments can be compared independent of their channel resolution [30].

### *2.3. 1D Fuel Spray Model*

Since the end of fuel injection occurred prior to the start of combustion in all injection timings studied, a 1D mixing-controlled inert Diesel spray model could be applied to predict such parameters as the maximum local fuel-air equivalence ratio at the start of combustion and the maximum free spray liquid length during the injection event [23,24]. The model has been developed to predict fuel spray behavior under transient conditions, such as a fuel spray into the combustion chamber of a Diesel engine during compression and expansion. One difference between the model and the engine combustion chamber is that the model has been designed to predict spray development in a large volume without wall effects, whereas the spray in the actual engine is affected by encountering combustion chamber surface areas (such as the piston bowl surface). These limitations of the model have been taken into account in this analysis and it should be noted that conclusions from the model are drawn on a qualitative basis, relative between each of the injection timings.

Based on the experimental test data entered into the 1D free spray model, the results are believed to quite accurately represent what was occurring in the actual engine tests. One of these inputs to the model is a description of the instantaneous mass flow rate of the fuel spray actually being injected into the combustion chamber. This information is derived from an experimental injection rate test with the actual engine, electronic controllers, and injection system inside the specific engine test cell [31]. The other input data set that the model requires is to generate the same environmental conditions in the model's large volume as in the engine. This data set includes details of the instantaneous in-cylinder pressure and density. This information is measured during the engine tests and prepared by a 0D thermodynamic code [32-34]. Based on these experimentally determined fuel spray mass flow rate and instantaneous in-cylinder conditions, the 1D free spray model can reliably calculate the in-cyinder fuel spray properties following each engine test.

## 3. Results and Discussion

### *3.1. Combustion Metrics*

It has been established that in-cylinder particle formation occurs in the regions of high temperature and local richness of the combustion chamber [17,18]. Therefore the first parameters analyzed were those which can readily indicate the quality of in-cylinder PM formation and oxidation (FIGURE 1). The first parameter used to predict the relative level of PM formation was the ignition delay (time from actual start of fuel injection to the start of the high temperature heat release), from a 0D thermodynamic analysis [32-34]. The second parameter, which came from the 1D free fuel spray model, was the maximum local equivalence ratio of the injected in-cylinder fuel at the start of the combustion (start of high temperature heat release) within the general combustion chamber volume. Both of these first parameters suggest the level of fuel-air mixing before the start of combustion (SOC). Therefore the longer the ignition delay, and lower the maximum local fuel-air equivalence ratio at the SOC, the lower the PM formation should be (for similar temperature conditions). The third parameter, adiabatic flame temperature after 85% fuel mass burned (Flame $T_{ad}$85), considers the level of in-cylinder PM oxidation. The higher the Flame $T_{ad}$85, the more particles that are presumed to have been oxidized during the combustion process.

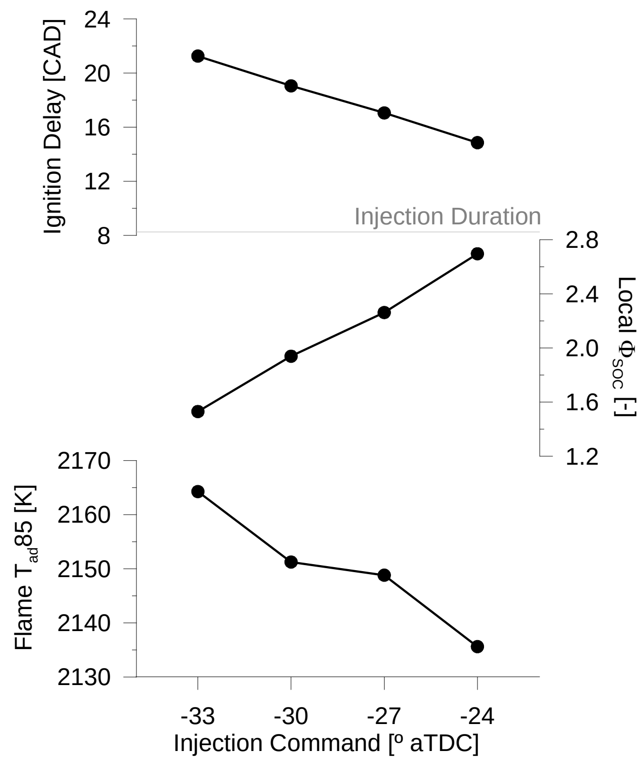


**FIGURE 1. Relative In-Cylinder PM Formation and Oxidation Metrics**

From FIGURE 1, it is possible to see that the ignition delay was longer than the injection duration in all injection timings studied. This means that the end of injection occurred before the start of combustion in all cases. Next seen was an increase in ignition delay and decrease in the local equivalence ratio at SOC with advances in injection timing earlier than -24°aTDC. Therefore, based on these two parameters, it can be presumed that in-cylinder PM formation should have decreased for earlier injection timings. Flame $T_{ad}$85 is shown to have increased with earlier injection timings. This suggests higher in-cylinder PM oxidation rates, and also supports decreased engine-out PM mass emissions with fuel injection timing advances earlier than -24°aTDC. Engine-out PM mass emissions are mostly based on the amount of particles formed minus the amount oxidized. Therefore these three parameters shown in FIGURE 1 suggest further decreases in engine-out PM emissions with advances in injection timing because of both lower PM formation and higher PM oxidation.

*3.2. General Emissions*

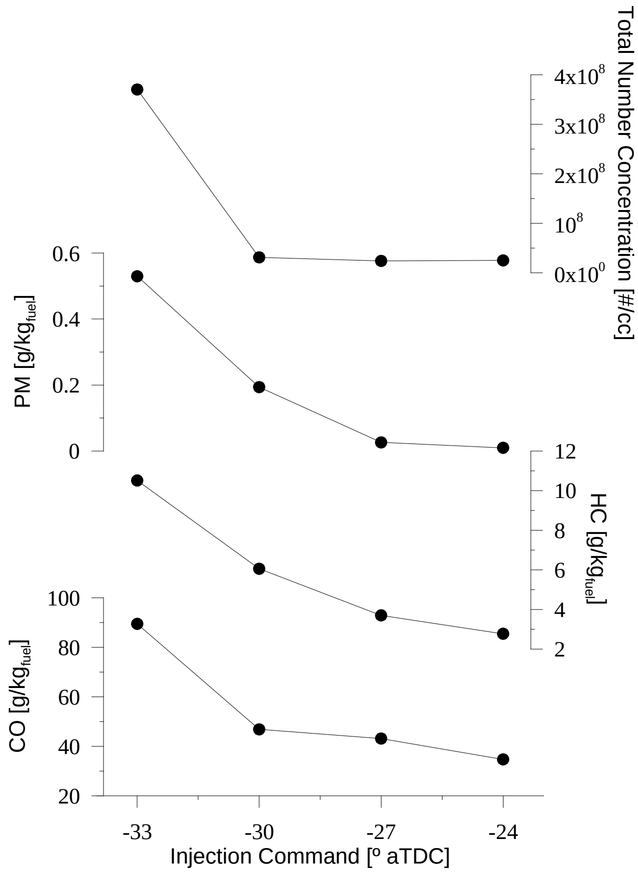


**FIGURE 2. Particulate Matter, Hydrocarbon, and Carbon Monoxide Emissions**

FIGURE 2 shows the emissions measurements for injection timings advanced of -24°aTDC (the injection timing of minimum PM early LTC). The values are represented in grams of emission specie per kilograms of fuel injected. This emissions index has the advantage that it is not subject to the changes in engine power at the different injection timings. Further advances in injection timing showed increased PM mass, PM number, HC, and CO emissions. One can see a much higher increase in PM number emissions (>11 fold increase) from -30 to -33°aTDC than the relative increase in PM mass (>2 fold increase). Injection timing wasn't advanced past -33°aTDC due to elevated in-cylinder pressure rise rates (>22 bar/CAD).

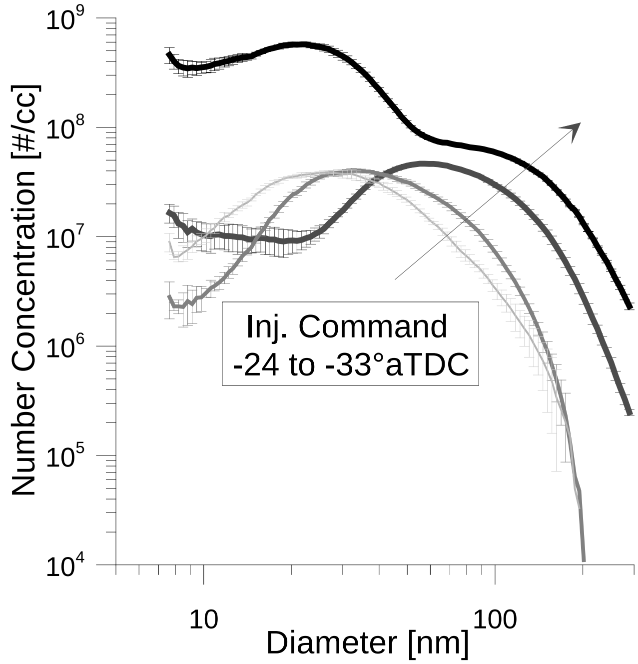


**FIGURE 3. Particle Size Distributions of Tested Injection Timings**

The particle size distributions of the PM emissions for the injection timings tested are displayed in FIGURE 3. A correlation can be seen between increased PM mass emissions and increases in number of particles larger than 50nm in FIGURE 2 and FIGURE 3. The large increase in total particle number concentration from the -30 to -33°aTDC injection timing (half an order of magnitude) in FIGURE 2 can be understood from not only the increase in particles larger than 50nm, but also the even larger increase in particles smaller than 50nm in the -33°aTDC injection timing. Montajir, et. al. proposed a conceptual model of the characteristics of the particles in the Diesel PM particle size distribution [13]. They proposed that the particles of the accumulation mode (particles larger than approximately 50nm) are primarily soot aggregates, conventionally produced in the locally fuel-rich/high temperature region inside a diffusive (mixing-controlled) Diesel flame. Although the PM formation and oxidation metrics from FIGURE 1 predicted a decrease in engine-out PM, and that all combustion cases investigated were completely pre-mixed combustion (no diffusive Diesel flame), the actual emissions measurements from FIGURE 2 and FIGURE 3 showed increased PM emissions with advances in fuel injection timing. Possible explanations of this contradiction between combustion metrics and PM measurements will be discussed in the next section.

*3.3. Investigating the PM Contradiction*

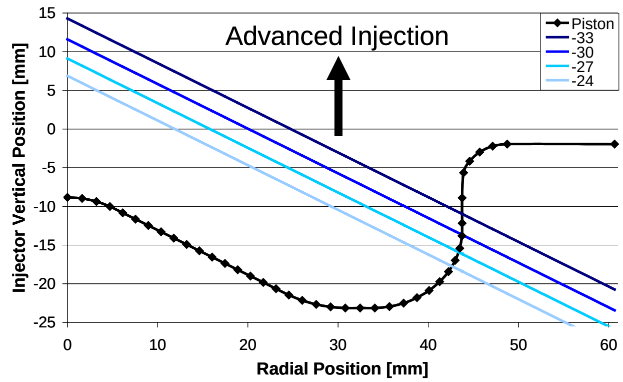


**FIGURE 4. In-Cylinder Fuel Spray Trajectory**

FIGURE 4 shows the trajectory of the fuel spray at the start of injection for each injection timing analyzed, projected onto the in-cylinder piston bowl surface. For advances in injection timing, the fuel spray trajectory crosses the piston bowl surface at a higher point (closer to the piston bowl lip).

It is believed that advances in injection timing increased liquid fuel deposition on the piston bowl surface, caused by increased liquid fuel spray – combustion chamber surface interaction, thus increasing engine-out PM emissions. Increased in-cylinder PM formation from increased fuel deposition on the combustion chamber surface has been observed by in-cylinder optical measurements [35-38].

One way to investigate the relative level of fuel deposited on the piston bowl surface between each injection timing is to compare the maximum free spray liquid length (from the 1D free spray calculation) attained during the injection event for each injection timing to the distance from the injector nozzle to the piston bowl surface at that moment. The 1D free spray model is capable of approximating the vapor spray length as well as the internal liquid spray length. Therefore analysis was performed using the maximum liquid spray length attained during the injection event and compared to the distance of the piston surface from the injector nozzle at that moment. The liquid overshoot shown in TABLE 3 approximates the length by which the maximum liquid length surpassed the piston bowl surface. This "overshoot" was calculated by subtracting the distance between the injector nozzle and the piston surface (at the instant of maximum liquid length) from the maximum liquid spray length predicted by the 1D free spray model.  The liquid overshoot length can then be qualitatively representative of the liquid fuel deposited on the piston bowl surface.

**TABLE 3. Maximum Liquid Spray Length Overshoot Past Piston**

| Injection Command [°aTDC] | -24 | -27 | -30 | -33 |
|---|---|---|---|---|
| Free Spray Maximum Liquid Length [mm] | 56.0 | 62.6 | 69.1 | 80.1 |
| Distance to Piston* [mm] | 45.9 | 47.6 | 48.8 | 49.1 |
| Liquid Overshoot [mm] | 10.1 | 15.0 | 20.3 | 31.0 |

*Distance to piston is the distance from the injector nozzle to the piston bowl surface at the instant of maximum liquid spray length.

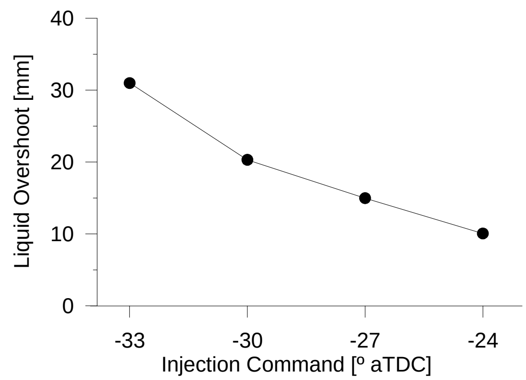


**FIGURE 5. Correlation of Liquid Spray Overshoot with Emissions**

In FIGURE 5, increased liquid fuel spray overshoot past the piston bowl surface correlated with increased PM mass, PM number, HC, and CO emissions.  Recalling that the requirements for PM formation are local fuel-richness and high temperatures (such as during the combustion process), this supports the idea that there was increased fuel deposition on the piston bowl surface for advances in injection timing earlier than -24°aTDC.  Even at the -24°aTDC injection timing, there appeared to be some liquid fuel deposition on the piston bowl surface predicted.  Although liquid fuel deposition on the piston bowl was predicted, the engine-out PM emissions were still very low.  Therefore it is proposed that the combustion process was still able to sufficiently vaporize, mix, and oxidize the relatively smaller amount of fuel deposited on the piston bowl in the -24°aTDC injection timing condition. But further liquid fuel deposition on the piston bowl may have been too much to vaporize and mix before the SOC, thus contributing to the in-cylinder PM formation. This increased level of liquid fuel deposition resulted in increased PM mass, PM number, HC, and CO emissions.

It is interesting to note that liquid overshoot increased by approximately 5mm for every 3 CAD advance of the injection timing from -24 to -30°aTDC. But the increase in liquid overshoot from -30 to -33°aTDC was much higher than the other injection timing intervals (approximately 8.7mm). From FIGURE 5 this higher increase in liquid overshoot from -30 to -33°aTDC compared well to the higher increase in total particle number concentration, PM mass concentration, HC, and CO than between the other injection timings.

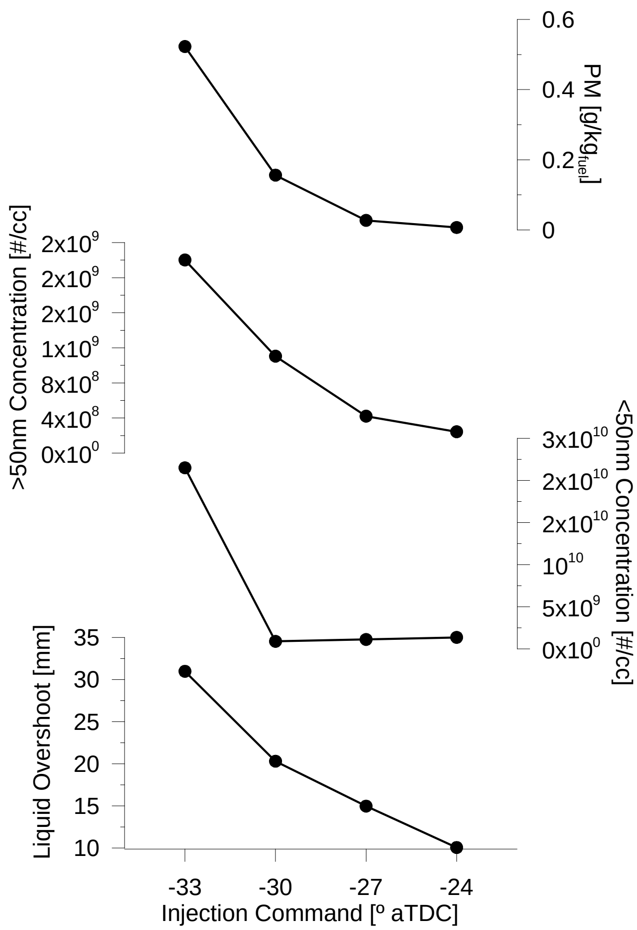


**FIGURE 6. Comparison of Liquid Spray Overshoot to Particle Mass and Number Concentrations**

FIGURE 6 shows a comparison of liquid overshoot and PM emissions (by mass and number concentration). The axis “>50nm Concentration” shows the sum of all channels for particles larger than 50nm, normalized to dN/dlogDp particle concentration. The axis of “<50nm Concentration” is likewise the sum of all dN/dlogDp normalized particle concentration channels smaller than 50nm. As seen earlier in the particle size distributions, the total PM mass concentration correlates well with the number concentration of particles larger than 50nm for advances in injection timing. This suggests, in agreement with Kittelson [12], that the particles in the accumulation mode (typically larger than 50nm) have a larger influence on the total PM mass concentration than the particles smaller than 50nm. Montajir, et. al. have suggested that the accumulation mode of the size distribution is typically composed of aggregate particles which are typically formed in the high temperature and locally rich regions of a mixing-controlled, diffusive Diesel flame [13]. As displayed in FIGURE 1, the end of injection occurred a few crank angle degrees (CAD) before the start of combustion in all injection timings analyzed in this study. This means that for these LTC engine operating conditions, there wasn’t believed to have been an injected-fuel mixing-controlled diffusive Diesel flame to form soot aggregate particles. But the particle size distributions showed increased emissions of large accumulation mode particles (typically classified by Diesel PM researchers as soot aggregates) with advanced injection timings. Therefore it is proposed that although the fuel injection had finished, soot aggregate particles still indeed formed in a mixing-controlled difussion flame at these early injection timings. In these engine operating conditions, the aggregates are suggested to have come from a low mixing energy diffusion flame that existed on the piston bowl surface where liquid fuel had been deposited during the earliest injection timings. This diffusion flame on the piston bowl surface would be less-optimal than a conventional Diesel mixing-controlled diffusion flame because of the piston surface that would block air entrainment into the flame (thus preventing reduction of the local richness in the high temperature regions of the flame). The diffusion flame on the piston bowl surface would also suffer from a great lack of turbulent mixing energy which is provided in the case of a conventional Diesel diffusion flame from the injected fuel’s spray momentum.

The formation pathway of the particles smaller than 50nm is more difficult to understand than of those larger than 50nm. Based on [12,13], the nucleation mode particles (typically smaller than 50nm) are largely composed of volatile material and can contain greater than 90% of the particle numbers. Looking at the increased HC emissions in FIGURE 2, it is suggested that there was an increase in engine-out condensable HC material which can contribute to the strong increase in particle emissions smaller than 50nm in the -33°aTDC injection timing. Kashdan et al. discussed the possibility of liquid fuel deposited on the piston bowl surface to flash boil during the expansion and exhaust strokes when the exhaust valve is opened [39]. But the very large increase in particle numbers smaller than 50nm from -30 to -33°aTDC didn't proportionally correlate to an equally larger increase in the liquid overshoot or overall HC emissions relative to the changes between the other injection timings. Therefore it is suggested that there were other factors not examined in this study, or more specific within the ones discussed, which contributed to the very large increase in particles smaller than 50nm from the -30 to -33°aTDC injection timing. But it remains true that the number of particles larger than 50nm did change similarly to the change in the liquid overshoot for all injection timings.

### *3.4. Methods of Liquid Length Reduction*

Some possible ways to decrease the HC, CO, and PM emissions by reducing the fuel spray's liquid length and fuel deposits on the piston are discussed in this paragraph. Increasing the engine's intake temperature, and therefore increasing the engine's in-cylinder unburned gas temperatures as well, would increase fuel vaporization and therefore reduce the injected fuel spray's liquid length. But higher intake temperature would also cause the injected fuel to auto-ignite earlier and decrease the ignition delay. As seen in FIGURE 1 and FIGURE 2, decreased ignition delay would decrease the time for fuel and air premixing before combustion, thus increasing PM formation.

A way to decrease the fuel spray's liquid length while maintaining approximately the same ignition delay would be by increasing the in-cylinder charge air density, achieved by increasing the engine's intake pressure. The effect of intake pressure on the particle emissions within the premixed Diesel LTC regime was further analyzed in [40]. But to maintain the same engine intake oxygen concentration or global combustion air/fuel ratio, an increase in EGR rate would be necessary. Since premixed LTC is currently limited to low to mid engine loads, it is already difficult to provide the exhaust turbine of the engine's turbocharger with enough exhaust gas energy to power the intake air compressor to generate moderate levels of intake air boost at these low loads. Depending on the engine, this option may not be possible simply due to turbocharger restrictions.

A final suggestion to decrease the fuel spray's liquid length would be by decreasing the injector nozzle's orifice diameter to increase air entrainment into the spray. While many orifices of small diameters would be interesting for completely premixed LTC (typically only applicable at low engine load conditions) since the injection finishes before the start of combustion, this injector nozzle design could be less advantageous for conventional diffusive mixing-controlled Diesel combustion (which has been proven to function throughout all engine loads and speeds).

**4. Conclusions**

Particulate matter mass and number emissions were shown to increase with further advances in the fuel injection timing earlier than -24°aTDC (the early injection timing with <0.05 FSN) within the Diesel LTC regime, contrary to increased ignition delay and $T_{ad}85$. These increases in PM emissions were also contrary to expected PM emissions decreases, based on the reductions in maximum local fuel-equivalence ratio predicted with advanced injection times by the free fuel jet spray model. Using a 1D free spray model, it was shown that increased PM mass, particle number, HC, and CO emissions with advanced fuel injection timings corresponded with higher relative levels of predicted liquid fuel deposition on the piston bowl surface. Therefore it is believed that the increased number of particles larger than 50nm (and even higher increase in particles smaller than 50nm) with further advances in injection timing past -24°aTDC in this LTC operating condition were due to increased amounts of fuel deposited on the piston during the injection process. This is especially attested by the increases in predicted fuel liquid spray overshoot and the increase in the particles larger than 50nm typically formed in the locally rich, high temperature regions of a diffusive Diesel mixing-controlled flame. Ways to reduce particulate emissions from liquid fuel deposition on the piston bowl surface included: increased engine intake temperatures to enhance fuel spray vaporization, increased intake pressure to reduce fuel spray liquid length without greatly reducing ignition delay, or by improved air entrainment into each fuel jet by smaller injector nozzle orifice diameters.

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