

Understanding Hydrocarbon Emissions in Heavy Duty Diesel Engines Combining Experimental and Computational Methods

Chad Koci, Adam Dempsey, Jeffery Nudd, and Bradley Knier
 Caterpillar Inc.

ABSTRACT

Fundamental understanding of the sources of fuel-derived Unburned Hydrocarbon (UHC) emissions in heavy duty diesel engines is a key piece of knowledge that impacts engine combustion system development. Current emissions regulations for hydrocarbons can be difficult to meet in-cylinder and thus after treatment technologies such as oxidation catalysts are typically used, which can be costly. In this work, Computational Fluid Dynamics (CFD) simulations are combined with engine experiments in an effort to build an understanding of hydrocarbon sources. In the experiments, the combustion system design was varied through injector style, injector rate shape, combustion chamber geometry, and calibration, to study the impact on UHC emissions from mixing-controlled diesel combustion. A tracer-based visualization methodology, using full cylinder and full cycle CFD simulations was developed to understand combustion chamber exhausting processes and help interpret crank-angle resolved test measurements of UHC in the exhaust runner using a Combustion Fast Flame Ionization Detector. Comparisons of the quantitative CFD predictions of UHC for varying engine configurations gives additional insight on the current state of the art predictive capability. Simulations with imposed fuel injector dribble phenomenon were additionally evaluated. The historical view of diesel UHC emissions having a strong dependency on injector dribble and injector sac volume was confirmed to still be of utmost importance. Results indicate that fuel injector dribble is a key source contributing from 75 to 90% of the UHC emissions under the conditions investigated. A discussion of simulation gaps and future modeling needs specific to diesel hydrocarbon sources highlights CFD capabilities required for research and development environments.

CITATION: Koci, C., Dempsey, A., Nudd, J., and Knier, B., "Understanding Hydrocarbon Emissions in Heavy Duty Diesel Engines Combining Experimental and Computational Methods," *SAE Int. J. Engines* 10(3):2017, doi:10.4271/2017-01-0703.

INTRODUCTION

The heavy-duty diesel engine is the primary power source for many markets around the globe such as transportation, mining, construction, agricultural, electric power generation, and the oil and gas industry. The diesel engine has undergone massive research and development over the past several decades in an effort to meet strict emissions regulations which have been implemented world-wide in both on-highway and off-highway markets. In 1996, the Tier 1 offroad regulations for diesel engines between 130 and 560 kW in the United States was 9.2 g/kWh for NOx and 0.54 g/kWh for soot. In 2014, the Tier 4 regulations were reduced to 0.4 g/kWh for NOx and 0.02 g/kWh for soot, which is a nearly 100% reduction in both NOx and soot emissions over the last two decades [1]. Thus, the primary focus of research and development has been on NOx and soot emissions reductions for diesel engines over the last two decades. The solution adopted by most diesel engine manufactures is a combination of optimized combustion system designs with moderate levels of exhaust gas recirculation (EGR) and aftertreatment, which includes a diesel particulate filter (DPF) and a selective catalytic reduction (SCR) device.

A significant amount of research has been conducted to understand the sources of NOx and soot emissions from diesel engines using optical engine experiments and computer modeling [2, 3, 4].

Additionally, researchers have been evaluating alternative combustion strategies such as low temperature combustion (LTC) to reduce NOx and soot emissions in-cylinder [5, 6, 7]. These LTC strategies, while reducing NOx and soot emissions in-cylinder, tend to increase unburned hydrocarbon (UHC) and carbon monoxide (CO) emissions. Thus, there has been some research into building an understanding of the sources of UHC emissions from diesel LTC strategies [8, 9, 10, 11, 12, 13]. However, there has been less research to understand the dominant sources of UHCs from modern heavy-duty diesel engines with relatively high engine out NOx and soot emissions that use a DPF and SCR to meet emission mandates. This is primarily due to the fact that the UHC emissions from these types of diesel combustion systems are generally low, on the order of 100 ppm at low load and 50 ppm at high load or less, and thus has not received as much research attention.

Historically, the conventional thinking of the main sources of hydrocarbon emissions from diesel engines are as follows [14]:

1. Overmixing (Lean): Overmixing of fuel and air creates regions that are too lean to combust to completion due to low combustion temperatures and results in UHC emissions. These regions are typically formed during the ignition delay period for diesel engines.

2. **Undermixing (Rich):** Undermixing of fuel and air creates regions that are too rich and result in UHCs due to insufficient oxygen. These regions are formed in the core of the fuel jet, from poor liquid atomization at the end of injection, from fuel injector dribble, and when liquid impinges on surfaces (e.g., pool fires). Liquid impingement is not likely for large bore engines, particularly at higher engine loads.
3. **Quenching:** Quenching occurs when a combusting spray impinges on a cold combustion chamber surface, such as the piston bowl, cylinder head, or the liner. High temperature reactions are quenched, resulting in UHCs.
4. **Misfire:** Misfire results in large amounts of hydrocarbon emissions. This is traditionally more of an issue with cold start and not typically a source of UHCs for well operating diesel engines.

Previous work by Matsui et al. [15] attempted to understand the dominate sources of UHC emissions from small bore, <100mm, diesel engines. They observed that flame quenching due to heat loss near cold surfaces was only a source of UHCs at low engine loads, even in a small bore engine that has a significant amount of spray/wall interaction. The other dominate sources persisted at all engine loads and included: overleaning during the ignition delay period, liquid fuel wetting on the piston bowl, and poor liquid atomization at the end of injection.

Yu et al. [16,17] studied the sources of UHCs from larger bore diesel engines and had similar findings with the exception that fuel wall wetting was not a dominate source of UHCs in the larger engine. Yu et al. observed that overmixing during the ignition delay period is a dominate UHC source and developed empirical correlations based on mixing rate, combustion lean limit, and other operating conditions. They also concluded that at high load with advanced injection timing, poor end of injection atomization and nozzle sac dribbling are dominate UHC sources. Additional work by Kuo et al. [18] continued to support the initial findings of overmixing during ignition delay and spray overpenetration as significant UHC sources with gas-jet modeling.

As hydrocarbon emissions regulations continue to tighten, large bore diesel engines are starting to require diesel oxidation catalysts (DOC) to meet UHC emissions mandates, which can be costly from a financial standpoint and an engine packaging standpoint. Therefore, with the ultimate goal of designing a combustion system that can meet UHC emissions regulations in-cylinder, there is a need to understand the sources of UHCs from heavy-duty diesel engines. The main focus of this work is to use single cylinder engine experiments and CFD modeling to build an understanding of the sources of hydrocarbons from large bore diesel engines with relatively low engine out UHC emissions, on the order of 100 ppm or less. The experiments used multiple engine out measurements of UHC emissions including a slow flame ionization detector (FID), a fast crank angle resolved (FID), and Fourier transform infrared spectroscopy. The CFD modeling included full four-stroke cycle simulations with valve motion, engine breathing, and combustion. Additionally, the CFD modeling used a novel region tracer methodology for tracking different portions of the combustion chamber during the exhaust stroke. The region tracer simulations facilitated a better understanding of the fast FID measurements by

pointing out which regions of the combustion chamber are likely responsible for distinct portions of the fast FID trace. The major findings of this work are as follows:

1. For the combustion systems investigated, the UHC sensitivity to engine calibration parameters such as injection timing, injection pressure, air/fuel ratio, etc., was only $\pm 15\%$. This level of sensitivity is low and points to the combustion system design as having an inherent source of UHCs that needs to be understood.
2. The shape and magnitude of the measured transient evolution of UHCs in the exhaust port was significantly different between two different fuel injectors. This suggests the UHC emissions can be impacted significantly by combustion system design, more so than engine calibration.
3. The CFD simulations using passive region tracers demonstrated that regardless of the tracer initialization time, the region near the firedeck is responsible for a large initial pulse of mass into the exhaust port (i.e., blowdown) followed by the cylinder core region. This finding was important for understanding the fast FID measurements.
4. The fast FID measurements for both combustion systems showed a large initial pulse of hydrocarbons followed by either a slow decay or a distinct second pulse depending on the combustion system design. The CFD simulations rather conclusively show that the first pulse stems from the near firedeck region.
5. CFD simulations with imposed fuel injector dribble demonstrated that the measured fast FID tracers can accurately be reproduced in both magnitude and shape. Thus, based on this work, a fuel injector dribble model is needed in the diesel engine simulation community to accurately predict UHC emissions from modern diesel engines. The fuel injector dribble model will also be critical for combustion system design simulations to aid in evaluating what designs consume the dribbled fuel and thus reduce engine out UHC emissions.

METHODOLOGY AND SETUP

The experimental methodology for the present UHC work centered on Single Cylinder Test Engine (SCTE) experiments. Two SCTE platforms were used and had a large variation in displaced volume, a Cat® 3500 based platform and a C15 based platform. Nominal geometric specifications for the two engines are listed in Table 1 with nominal displacements of 5L/cylinder and 2.5L/cylinder. Most of the work presented here will focus on the 3500 SCTE with the C15 SCTE being used for historical data and simulation perspectives.

Table 1. Single Cylinder Test Engine Specifications

	3500	C15
Displaced volume	4.88 L	2.53 L
Bore	170.00 mm	137.19 mm
Stroke	215.00 mm	171.45 mm
Connecting Rod	392.50 mm	270.76 mm
Compression ratio	15.5:1	16.8:1
Injector	Common Rail or Mechanical Injection	

The 3500 SCTE operation conditions were based on the Off-Road Type C1 steady-state certification cycle 8 mode points (ISO 8178). Emissions standards of interest would correspond to off-road engines greater than 560 kW for the 3500 and between 130-560 kW for the C15. An example of the 8-mode points for the 3500 are listed in Table 2 where the rated power speed is 1800 rpm and the intermediate speed is 1350 rpm. The present work used very similar modal points for UHC investigation, although some modes were not as heavily evaluated as others.

Table 2. Off-Road C1 steady-state certification cycle example for an engine with >560 kW rated power.

Mode	Power	Speed	Torque	BMEP	Torque Percent	C1 Cycle Weighting
-	kW	rpm	Nm	kPa	%	-
1	1863	1800	9884	2121	100%	0.15
2	1397	1800	7413	1591	75%	0.15
3	932	1800	4942	1060	50%	0.15
4	186	1800	988.4	212	10%	0.1
5	1411	1350	9978	2141	100%	0.1
6	1058	1350	7483.5	1606	75%	0.1
7	705	1350	4989	1071	50%	0.1
8	10	700	135	29	0%	0.15

Diagnostic Setup

Measurement of diesel UHC was completed with three different types of engine emissions analyzers: Emissions bench Flame Ionization Detector (FID), Fourier Transform Infrared (FTIR) spectrometer, and Fast FID. The Emissions bench was model Horiba MEXA 7100D calibrated with normal engine certification procedures. The FTIR was model MKS 2030HS setup to sample at the same location as the Horiba emissions bench, which is downstream of the exhaust surge tanks and the backpressure valves on the SCTE. The Fast FID was a Combustion HFR500 setup to sample crank angle resolved UHC concentrations from the exhaust port.

Since traditional FID and FTIR measurements are commonplace in the engine industry, the details of the setup and analyzer accuracy will be omitted. However, it should be noted that a challenge exists with sample location and exhaust residence time, particularly for SCTEs like the one used in this study. It is known that substantial UHC oxidation can occur in the exhaust system if the residence time and temperature are sufficient, much like that of SCTE setups with large exhaust plenums/barrels when operated at sufficient load. Due to this UHC exhaust system oxidation concern, care must be taken to reasonably account for the effect. Figure 1 shows the correction factor correlation that was used in this work. The correlation was derived from a 3500 multi-cylinder test engine (MCTE) running the same conditions as the 3500 SCTE. The MCTE has very little exhaust residence time relative to the SCTE. The SCTE and MCTE had very similar UHC emissions for exhaust temperatures less than 400° C. For exhaust temperatures higher than 400° C, they began to deviate with the MCTE having higher UHC emissions. Thus an empirical correction factor was applied by using the difference between the MCTE and SCTE datasets above 400° C exhaust temperature.

One of the novel aspects of the current experimental work was the use of a Fast FID to gain crank angle resolved measurements of UHC emissions. The Fast FID measurements were challenging due to the precise nature of the HFR500 and high-contaminant (soot/PM) exhaust stream of diesel engines. Soot/PM fouling was evident by observations of increased (>10%) FID concentration-to-voltage gain with post-test calibration (propane used as calibration gas) prior to post-test cleaning. Data quality was maintained to eliminate points with unacceptable FID head gain changes. Fast FID measurements were limited to less than 50% load due to sampling flow limits and analyzer probe temperature limits at higher loads. The higher exhaust pressures (>400 kPa abs) at the higher loads were found to be problematic as well. A regular calibration and cleaning methodology was used daily to ensure reliable operation over the test campaign. The HFR500 has a listed T90-10% response time of 0.9 to 1.3ms and accuracy of < ±1% of full scale.

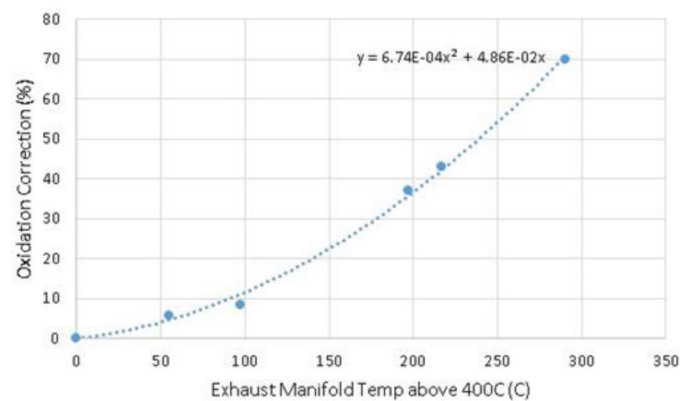


Figure 1. Emissions bench FID oxidation correction applied to account for in-exhaust system UHC oxidation effects with high residence time and temperature, which is experienced on the SCTE relative to the MCTE.

The Fast FID analyzer probe was installed on the sole exhaust runner of the single-cylinder 3500 at a position just outside the mating surface of the cylinder head and exhaust runner, approximately 25 mm outside the cylinder head. The probe was centered in the runner to sample the core of the exhaust flow. No probe location sensitivity study was performed on probe position for the present work.

The Fast FID data was acquired with the other high speed crank angle resolved measurements, such as cylinder pressure, at 0.1 CAD resolution. Processing of the Fast FID signal was completed with a MATLAB® routine which performed the following operations:

- Processed each engine cycle (usually 300)
- Time shifted the data to account for transport through the sampling line and sensor response delay
- Base delays were ~3ms for the 150 mm probe determined through initial data analysis
- The base time delay was adjusted to account for exhaust runner pressure effects on probe transport time
- Calculated the mass flow of UHC from the concentration Fast FID data and 1D engine simulation exhaust mass flow profiles based on operating conditions



- Integrated each cycle's UHC mass flow and discarded the highest 10-20%, representing outliers from soot interference in the measurement. This process will be described in a subsequent section.
- Reported final UHC vs. CAD average signals and an exhaust mass average ppmC1 UHC measured by the fast FID for comparison with other measurement techniques.

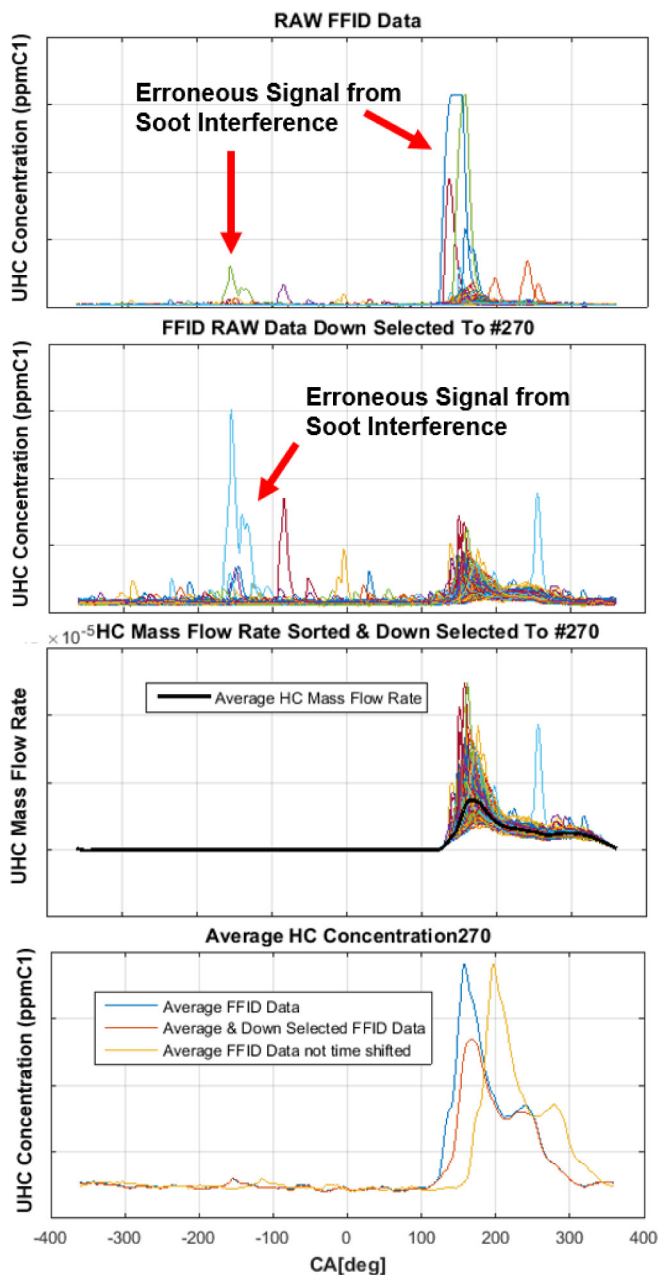


Figure 2. Example of Fast FID data processing result from 300 cycles of diesel engine data. The highest 10% or 30 mass cycles were thrown out (hence down selected to 270) to eliminate bias introduced from erroneous high cycles which contain soot signal interference.

An example of the Fast FID raw and processed data can be seen in Figure 2 over the four line plots. The raw data is cleaned and time-shifted to produce the best estimate of the actual UHC time-history without soot interference. The average signal is significantly affected when there is soot ingested into the FID as seen in the lowest

plot in the figure by comparing the average with and without down selecting. The general shape of the UHC signal does not change, but the magnitude of the time-resolved features do change when the high-soot cycles are removed from the ensemble averaging. Engine cases with higher soot showed an increase in the amount of erroneous signal, easily identifiable through this processing method. Some cases required more than 10% removal due to the higher soot. The removal of the highest integrated mass curves does change the cycle-to-cycle UHC distribution, but it was the best method found to consistently and quickly remove the large erroneous signal from soot.

3D CFD Simulation

CFD modeling of selected engine test points was completed to help better understand the UHC emissions sources from these heavy-duty diesel engines. CFD models of diesel combustion were built in CONVERGE® v2.2 using well-stirred reactor combustion models with detailed n-heptane chemistry, RNG k-ε RANS turbulence modeling, Lagrangian spray modeling, and physical fuel properties of US diesel. Full 360° engine combustion chamber geometry was used in conjunction with engine intake flow simulations to initialize flow fields at IVC. An example full-geometry domain of the 3500 SCTE can be seen in Figure 3. Combustion simulations were completed for the closed portion of the cycle from IVC to EVO. Subsequent exhaust simulations were completed from EVO to EVC or the combustion simulations were continued all the way from IVC to EVC. Minimum cell sizes were below 0.5 mm in areas of the spray and high temperature and velocity gradients, resulting in simulations with millions of cells, using 2000-10000 core-hours per case depending on engine size and simulation crank angle period. High-quality boundary condition data was available for the present data sets from the single-cylinder engine experiments coupled with 1D cycle simulation modeling. Fuel injector rate shape characterization came from Caterpillar's spray facilities, where momentum rate and delivery measurements provided accurate injection velocity profiles [19].

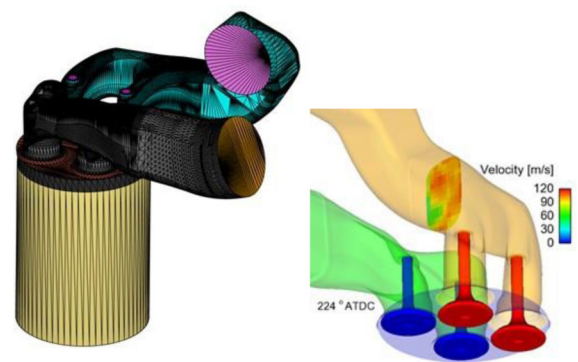


Figure 3. Example full-geometry Converge model domain including intake and exhaust ports.

3D Flow Simulation Methodology

CFD simulations were used to simulate the full 3500 engine geometry and study how and when different regions of the combustion chamber exhaust during the exhaust stroke through use of a passive tracer. The results of this methodology will aid in the ultimate goal of building an understanding of the sources of UHC

emissions. These CFD simulations will be used in conjunction with the temporal fast FID measurements to highlight the likely regions responsible for the UHC emissions.

Many approaches were considered such as pathline and streamline analysis. However, these approaches could have limitations when it comes to the required time step interval of output files. Additionally, this type of analysis is useful for flow visualization, but is not quantitative for the purpose of comparisons to the fast FID measurements. Instead, a passive tracer based analysis approach was used. Figure 4 illustrates the concept. Shown in the figure is fluid flowing from left to right over a bank of four cylinders, with the top half of the fluid dyed blue and the bottom half of the fluid dyed red. As the fluid flows over the cylinder bank, the two dyed regions begin to mix and are stretched and distorted due to fluid motion and turbulent mixing. The dyes are non-reactive and thus are not created nor destroyed, but simply change in local concentration by fluid motion and mixing. By examining a given fluid packet downstream it can be determined quantitatively what proportions of the fluid packet stem from the top and bottom halves of the initial incoming flow. This passive tracer approach was implemented into the CFD simulations to analyze what regions of the combustion chamber exhaust at what time.

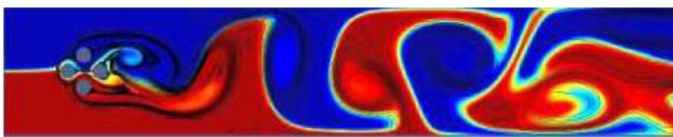


Figure 4. Example of the passive tracer methodology for tracking fluid flow behavior.

To begin the analysis in CFD, the modeled domain needs to be discretized into the regions of interest. This is done within the CONVERGE v2.2 framework by starting with a simulation map output file at the crank angle of interest from which the subsequent exhaust stroke simulation will begin.

The simulation map file contains the geometric location of each CFD cell in the domain and the properties of that cell. In this work two different crank angles will be investigated for initiating the nonreactive tracer species: EVO and near the end of combustion. For the 3500, EVO is 123.5° ATDC and the end of combustion for the mode 3 point (1800 rpm, 50% load) investigated is 46° ATDC.

The computational domain was first divided into an intake and exhaust side which is sectioned down the center of the cylinder, coincident with the centrally mounted fuel injector tip. Then, high level regions of interest were identified to be the injector tip region, the firedeck region, the squish region, the bowl region, and the cylinder core region. This resulted in 11 regions of interest within the CFD model of the 3500 which contained ~6.1 million cells at EVO. Based on user inputs of the region geometric boundaries (radial and z-location boundaries), a script finds and flags the CFD cells that reside in these regions at the starting crank angle of interest.

Figure 5 and Figure 6 show the resulting tracer initialization for 2 example regions: the injector tip and intake side squish region. Figure 5 shows the computational domain at 123.5° ATDC, which is EVO and the start of the exhaust stroke simulation. Figure 6 shows the domain at 46° ATDC, which is the end of combustion for the mode 3 point (1800 rpm, 50% load) investigated. As shown in the figures, the initial geometric locations of the tracer species are identical, except that the piston position tends to change the relative size of the regions that are not of a fixed thickness near the firedeck. When the tracer species are initialized at EVO, it allows the exhaust stroke to be studied and build and understanding of what regions of the combustion chamber exhaust at what time. On the contrary, when the tracers are initialized at the end of combustion, the resulting CFD simulation will provide insight into what regions the UHCs could be stemming from due to the fact that the UHCs will likely be frozen near the end of combustion.

It is important to understand and take note of the different initial region volumes for the different initialization times. As the region initialization time changes, and thus the piston location changes, the tracer regions that are not anchored to firedeck or the piston will change in size. These regions are the squish and cylinder core. The initial size of the other regions is unaffected by the tracer initialization time (i.e., injector tip, firedeck, and bowl). These concepts are illustrated in Figure 7. As shown, the injector tip, intake side firedeck, exhaust side firedeck, intake side bowl, and exhaust side bowl region volumes are not a function of the initialization time. They are constant. However, the intake side squish, exhaust side squish, intake side cylinder core, and exhaust side cylinder core have region volumes that are a strong function of the initialization time. Due to this, the 46° ATDC initialization time gives a more uniform distribution of region sizes compared to the 123.5° ATDC case. These differences will be important to understand and remember when digesting the tracer flowrate simulation results.

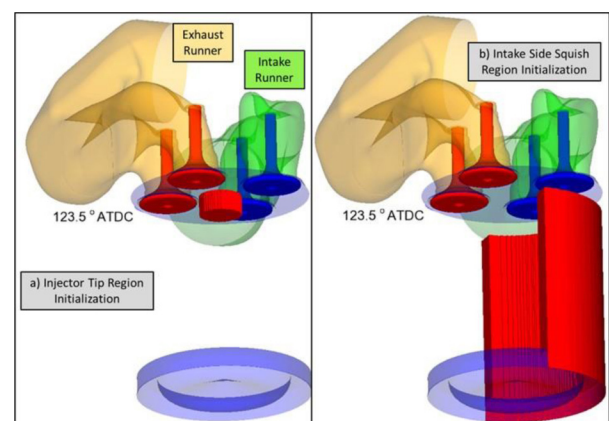


Figure 5. Example of tracer species initialization for the 3500 at EVO (123.5° ATDC) for a) the injector tip region and b) the intake side squish region.

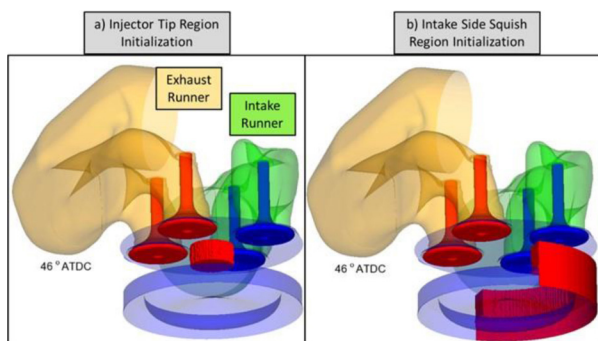


Figure 6. Example of tracer species initialization for the 3500 at end of combustion (46° ATDC) for a) the injector tip region and b) the intake side squish region.

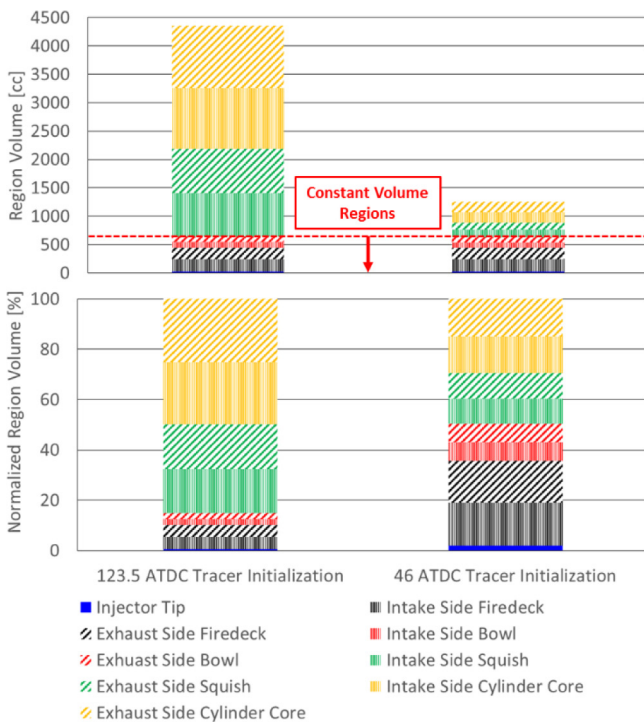


Figure 7. (Top) Tracer region absolute initial volume for the two initialization times. Red dashed line indicates that the regions below the line have a constant volume and are not a function of initialization time. (Bottom) Tracer region normalized volume percentage.

EXPERIMENTAL RESULTS

The experimental engine conditions investigated were nominally those outlined in Table 2 for the 3500. C15 investigations were primarily conducted at 1800 rpm over a few loads with a similar range to the BMEP in Table 2. Detailed Fast FID UHC measurements were more concentrated on Mode 3 for the 3500 due to challenges with full load measurements, as was discussed previously.

UHC Sensitivity to Engine Calibration

An understanding of the effect that calibration has on UHC emissions was desired using a baseline combustion system. The range of engine boundary conditions investigated to perturb the engine calibration for the 3500 at Mode 3 were:

- Injection Timing (main SOI from -10 to 10° ATDC)
- Injection Rail Pressure (120 MPa to 250 MPa)
- Injection Shot Mode (pilot, main, post, etc.)
- EGR (0 to 35%)
- IMAP (250-400 kPa)
- AFR (30 to 50:1)
- IMT (30 to 65 °C)

A $\pm 15\%$ total UHC sensitivity, with a total band width of 30%, is clearly seen in Figure 8 for all of the Mode 3 sensitivity data acquired. The Emissions Bench and Fast FID measurements show the same $\pm 15\%$ range, with the Fast FID having an offset lower. The FTIR data showed more variance, believed to be an artifact of the measurement technique and the FTIR algorithm for calculating total hydrocarbons. Again, these low levels of UHC emissions (10-200 ppmC1) are a challenging measurement with many considerations for calibration gas, calibration condition, sampling system, and unique instrumentation sensitivities. Generally, all three measurements of UHC showed consistent trending and sensitivity despite the absolute magnitude offsets, which are slight in their own regard.

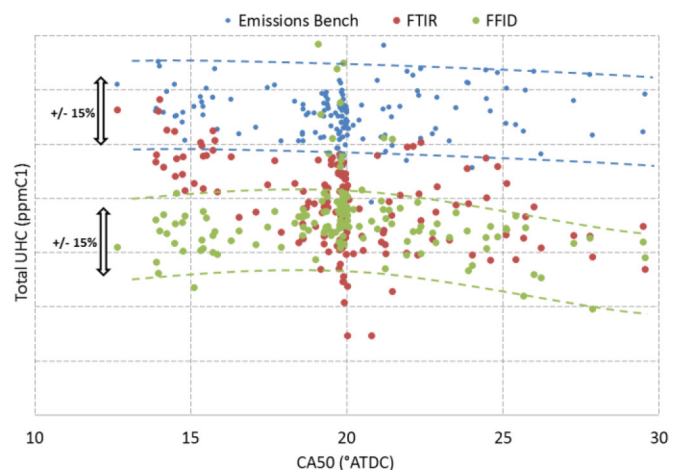


Figure 8. 3500 UHC sensitivity to engine calibration for Mode 3.

The fact that the baseline combustion system for the 3500 engine displays such a low sensitivity of UHC emissions to engine calibration changes of only $\pm 15\%$ is an interesting finding. This low level of sensitivity suggests that the combustion system design is the inherent source of UHC emissions that needs to be more fully understood.

Engine Hardware Variations

The UHC data for all of the 3500 experiments is presented in Figure 9. The data was taken such that at each engine mode the same air system boundary conditions (AFR, EGR, MAPs, IMT) were used between hardware variations. Hardware variations consisted of: fuel injector style, injector nozzle specifications, and piston bowl shape. Multiples of the same color/style data points at each mode represent different SOI and fueling variations completed at fixed AFR. The exact differences in data points are not disclosed due to confidentiality, but a baseline condition can be considered to be where the blue curve is drawn over the data points. The UHC plotted is the exhaust temperature corrected measurement from the