

Detailed Unburned Hydrocarbon Investigations in a Highly-Dilute Diesel Low Temperature Combustion Regime

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ABSTRACT

The objective of this research is a detailed investigation of unburned hydrocarbon (UHC) in a highly-dilute diesel low temperature combustion (LTC) regime. This research concentrates on understanding the mechanisms that control the formation of UHC via experiments and simulations in a 0.48L signal-cylinder light duty engine operating at 2000 r/min and 5.5 bar IMEP with multiple injections. A multi-gas FTIR along with other gas and smoke emissions instruments are used to measure exhaust UHC species and other emissions. Controlled experiments in the single-cylinder engine are then combined with three computational tools, namely heat release analysis of measured cylinder pressure, analysis of spray trajectory with a phenomenological spray model using in-cylinder thermodynamics [1], and KIVA-3V Chemkin CFD computations recently tested at LTC conditions [2]. This study looks at the effect of inlet oxygen concentration, fuel spray targeting, injection event timing, injector sac volume, rail pressure, and boost pressure which are each explored within a defined operation range in LTC. This research compliments simultaneous research which concentrates on understanding the benefits of multiple injections on engine performance and emissions operating in the LTC regime [3].

The results of this research show that total UHC can be divided into light (<6 carbon/molecule) UHC and heavy (≥ 6 carbon/molecule) UHC emissions. The light UHC closely track with CO having minimum exhaust concentrations on the order of 250 ppm and occur when CO is at its 0.5% minimum. Spray targeting, percent inlet oxygen, and boost pressure variation produce the largest light UHC changes, where as injection pressure has minimal effect. Liquid fuel injected outside the piston bowl, which can occur with early injection, is linked to the heavy UHC components where a 3 times increase is observed relative to later injections where the liquid stays within the bowl. Injector sac-volume experiments suggest the sac volume is a relatively constant source of heavy UHC and can contribute as high as 15% of the total UHC. Based on these results, a simple three-part UHC model is suggested and hypotheses are discussed for the over-rich dominant sources of the unburned hydrocarbons.

INTRODUCTION

Recent research suggests that UHC emissions during LTC result from the incomplete combustion of under-mixed fuel and charge gas occurring after the

premixed burn period [4, 5, 6]¹, or significant UHC emissions could be resulting from over-mixed regions at the end of fuel injection [7, 8]. Previous research has investigated CO trends in a highly-dilute LTC regime with less detail applied to the UHC trends. Upon close inspection the trends from Opat et al. [6] were very different, spurring questions which required further investigation and analysis. The objective of the present work was to increase understanding of the UHC emission mechanisms, and why they sometimes differ significantly from the CO emissions.

In order to continue usage of CI (Compression Ignition) combustion under current regulations, different approaches can be taken to lower the NO_x and PM emissions of conventional diffusion type combustion. Most of these techniques use some variation of injection timing and increased EGR to increase ignition delay. Some approaches also involve techniques to increase in-cylinder mixing. However, as these techniques are used to drive NO_x and PM emissions down sufficiently to meet the lowest future emissions regulations, UHC and CO levels increase beyond acceptable levels.

The highly-dilute Low Temperature Combustion (LTC) regime (similar to the work in [9]) requires very high EGR (>60%) in order to sufficiently prolong the ignition delay of the mixture and lower the mixture temperatures. This combustion is typically realized at global mixture compositions just lean of stoichiometric, as opposed to much leaner mixtures in conventional diesel combustion. Some of the various names which have been used to describe techniques involving LTC are Premixed Compression Ignition (PCI) [10], Premixed Charge Compression Ignition (PCCI) [11], Homogeneous Charge Compression Ignition (HCCI) [12], and MK [13]. However, HCCI would typically refer to a strategy where the fuel is injected extremely early, resulting in a nearly homogeneous mixture of fuel and air in the combustion chamber. PCI or PCCI, on the other hand, is typically achieved with less advanced injection timing (but more advanced than for conventional diesel) where the fuel is injected in the combustion bowl with the objective of providing a not only fully vaporized fuel cloud but also sufficiently mixed fuel and air within the combustion bowl to avoid significant soot formation. The MK strategy [13] uses relatively retarded injection timings to increase ignition delay and allow for pre-mixing. The strategies cited above can also be combined to enable broader coverage of the engine load and speed range [14].

In the Equivalence Ratio vs. Temperature space shown in Figure 1, it is evident how the requirement to achieve lower equivalence ratios using increased mixing and low temperatures simultaneously can reduce NO_x and Soot. Conventional diesel combustion travels through the Soot

and NO_x islands while LTC, PCCI and HCCI all narrowly avoid the high formation regions for these emissions. The shape and location of these islands is a function of the in-cylinder conditions particular to the operating point, but the general behavior remains similar over a range of conditions.

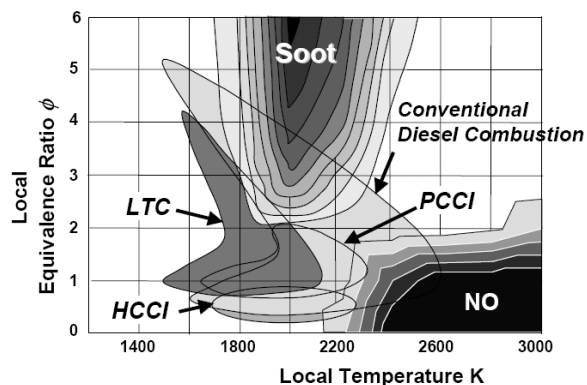


Figure 1: Modern diesel combustion strategies plotted in ϕ -T space [14].

Because of the overlap of these various advanced combustion techniques, for simplicity, the combustion strategies studied in this paper will be referred to simply as LTC. The use of this form of combustion is currently restricted to light loads based on the low cylinder temperature and pressures that are necessary to maintain the decreased NO_x. It is of great interest to push the current limits of LTC by going to higher loads and lower inlet oxygen levels. At these very low inlet O₂ levels, increased amounts of CO and UHC begin to appear along with increased combustion noise.

As discussed beforehand, when operating in LTC significant increases in UHC emissions are typically observed. The dominant source of the UHC emissions is under strong debate and is most likely dependent upon the engine operation condition. An illustration of this would be analogous to conventional diesel combustion where at light-load conditions in small displacement engines, over-mixing of air and fuel creating lean zones is one dominant source [15]. For LTC light-load applications additional UHC sources are believed to be important and include fuel liquid films, quenching zones, and under-mixed or fuel rich zones [16, 17, 18]. By taking a global view of these sources it is evident that all of the postulated UHC sources in LTC come from regions or situations where there are poorly mixed products and/or insufficient thermal energy to promote the oxidation kinetics. Clearly improved mixture preparation and thermal homogeneity would have great benefits on UHC emissions.

¹ Numbers in brackets designate references listed at end of paper

Figure 2 shows how the CO and UHC trends in an extremely dilute LTC condition (~67% EGR) do not track together across a SOIC (start of injection command) sweep. CO emissions are minimized near -33 °ATDC and have been shown to be dominated by mixing and spray-targeting phenomena. UHC emissions also show a minimum near -33 °ATDC, but show a much smaller increase as SOIC is retarded further. This observation suggests that UHC may be controlled by somewhat different mixing and spray-targeting phenomena than those which control the CO trends. This experimental observation initially instigated the present work, and an in-depth analysis into the differences is needed for a better understanding of the UHC emissions mechanisms.

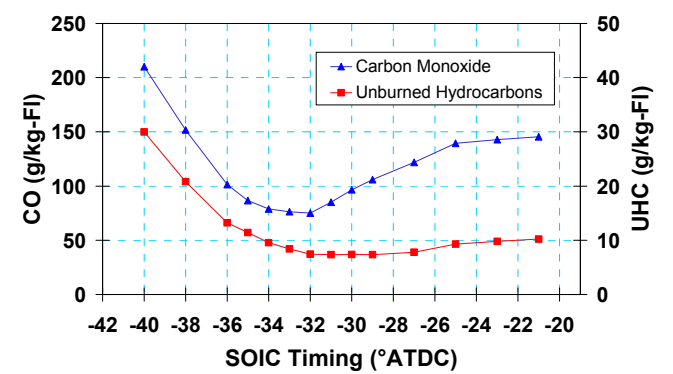


Figure 2: Differences in UHC and CO trends become apparent in LTC over a single injection SOIC sweep [19].

EXPERIMENT

ENGINE SETUP

The engine used to conduct this research is a single-cylinder version of a GM 1.9L, 4 cylinder light duty diesel engine; the specifications of which can be seen in Table 1. The production head and valve-train were used in conjunction with a Labeco CLR crankcase. A re-entrant bowl design with lower compression ratio than the current Euro-4 compliant production configuration was used along with a slightly longer connecting rod length; all other cylinder geometry was matched to the equivalent 4-cylinder engine. The single-cylinder engine has the capability to run up to 4000 RPM at full-power conditions using pressurized inlet air to simulate the behavior of a turbocharger. Full capability for variation of EGR rate, coolant and oil temperature and respective inlet and exhaust pressures and temperatures exists in the laboratory. Figure 3 shows the schematic of the engine and test cell layout.

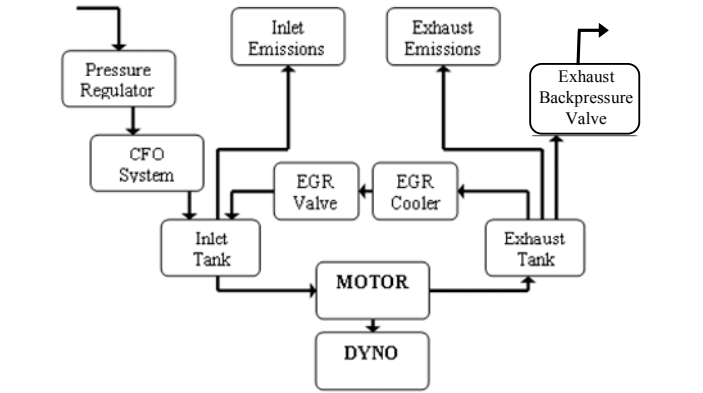


Figure 3: Schematic of test cell layout. CFO stands for Critical Flow Orifice.

Table 1: Engine Specifications

Displacement	0.4774 [L]
Bore	82.0 [mm]
Stroke	90.4 [mm]
CR	16.6:1
IVO	344 ° ATDC
IVC	-132 ° ATDC
EVO	112 ° ATDC
EVC	388 ° ATDC

The injection system utilizes a BOSCH CP3.3 pump for producing fuel rail pressure. The ETAS INCA calibration software used in conjunction with the production ECU allows for up to 5 injections per cycle. A production CRIP2-MI injector was used with an experimental 7 x 155° nozzle tip with a flow number of 440 cc/30sec, unless otherwise specified summarizes the injection system specifications.

The measurement of cylinder pressure data was accomplished via a piezoelectric KISTLER 6125B pressure transducer. The resolution of data was 0.1 CAD, corresponding to 3600 counts per revolution; 200 cycles of data were recorded for all heat release analysis. The combustion noise was recorded using an AVL Combustion Noise Meter (Model A01); meter output was in decibels.

Table 2: Injection System Specifications

Fuel Injection Equipment		
Design	<i>Common Rail</i>	-
Injector	<i>Bosch CRIP 2</i>	-
Included Cone Angle	<i>155*</i>	<i>Deg</i>
Nozzle Type	<i>Mini-Sac</i>	-
Nozzle Flow Number	<i>440</i>	<i>cc/30sec</i>
Nozzle Hole Diameter	<i>0.139</i>	<i>mm</i>
Number of Holes	<i>7</i>	-
Operated Rail Pressures	<i>860*</i>	<i>Bar</i>
Peak Rail Pressure	<i>1600</i>	<i>Bar</i>
Fuel Pump	<i>Bosch CP3.3</i>	-

*Unless otherwise specified in detail

The fuel used in the experiments was intended to be a typical US Ultra Low Sulfur Diesel (US-ULSD) with a Cetane of 42.9. The general properties of this fuel can be seen in Table 3.

Table 3: General fuel properties for testing

Fuel Properties for the Typical US-ULSD		
Spec Gravity	<i>0.847</i>	-
API Gravity	<i>35.64</i>	<i>API</i>
VISCOSITY @ 40 °C	<i>2.025</i>	<i>cSt</i>
HHV	<i>19571</i>	<i>Btu/lb</i>
HHV	<i>45.52</i>	<i>MJ/kg</i>
NON-AROMATICS	<i>66</i>	<i>% wt</i>
MONO-AROMATICS	<i>26.2</i>	<i>% wt</i>
PAH'S	<i>7.8</i>	<i>% wt</i>
Cetane number	<i>42.9</i>	<i>D613</i>
Temp at 50% Distilled	<i>237.8</i>	<i>°C</i>

Exhaust emissions were measured using a Horiba emissions bench capable of recording CO₂, CO, (Model AIA-220), O₂ (Model FMA-220), THC (Model FIA-236-1, propane span gas) and NO_x (Model CLA-220). Throughout the experiments NO_x emissions remained extremely low near 3-6 ppm for all cases. In addition, a reflectivity-based PM measurement was taken using an AVL Smoke Meter (Model 415S) at each operational point. The emissions sample was extracted downstream of both the exhaust surge tank and the exhaust backpressure valve. In order to obtain the real-time mass percentage of EGR, measurements on the same Horiba emissions bench were done for inlet CO₂ (Model AIA-210) and inlet O₂ (Model MPA-21A). A MKS FTIR (Model 2030HS) was used for increased hydrocarbon investigations and allowed for general classes of UHC species to be identified. All emissions equipment used heated lines and filters except the EGR CO₂ and O₂.

Table 4 lists the major combustion species identified in the experiments.

Table 4: FTIR Measurement Species of Interest

MKS FTIR Combustion Species	
Standard Combustion Species	<i>CO₂, CO, NO, NO₂, and H₂O</i>
Available Hydrocarbon Combustion Species	<i>Diesel*, Dodecane, Octane, Heptane, Toluene, Pentane, Butane, Propane, Propylene, Ethane, Ethylene, Acetylene, Formaldehyde, Methane</i>
<i>* Diesel is representative of C12 and higher from MKS empirical correlations</i>	

TEST CONDITIONS

The baseline LTC engine operational conditions can be seen in Table 5. The condition is very dilute utilizing a maximum of ~67% EGR based on the controlling parameter of the inlet oxygen concentration of 9.50% +/- .05%. The extremely dilute condition is required to observe mixing and fuel spray-targeting impacts on CO and UHC as documented by [1, 6]. For the baseline conditions the CO minimum, or "sweet-spot" (emissions-optimal edge of bowl targeting [6]), condition was at a single injection SOIC (start of injection command) timing of -33° ATDC. The reader should know that at 2000 rpm the listed SOIC timings are 4.8° advanced from the actual SOI timings.

Table 5: Baseline LTC Engine Operation Conditions

Engine Speed	<i>2000 rpm</i>
Engine Load	<i>5.5 Bar Net IMEP*</i>
Nozzle Angle	<i>155°</i>
Fuel Rail Pressure	<i>860 Bar</i>
Swirl Ratio	<i>2.2</i>
Inlet Pressure	<i>162 kPa abs</i>
Exhaust Pressure	<i>182 kPa abs</i>
Inlet O₂	<i>9.50%</i>
EGR	<i>~67%</i>
Intake Temperature	<i>65° C</i>
EGR Temperature	<i>45° C</i>
Coolant Temperature	<i>90° C</i>
Oil Temperature	<i>90° C</i>

* Net IMEP is defined as gross IMEP minus pumping MEP calculated from pressure-history data.

In these experiments both single injections and multiple injections were used. The investigated variables of EGR, single injection timing, inlet boost pressure, and

injection rail pressure are presented in Table 6. The split-injection timings for the EGR sweep from 0-67% were chosen to allow for the full range of EGR to be covered without running into combustion noise limits. Single injection SOIC sweeps were performed with the baseline operation conditions from -44° to -15° ATDC. Fuel injection pressures were varied from 600, 860, to 1120 bar along with inlet boost pressures varied from 142, 162, and 182 kPaa.

Table 6: Test case matrix. All injection timings are in °ATDC.

Test Variable	% EGR Sweep	Single Inject.	Inlet Boost	Rail Press
SOIC_1 st	-20°	-44° to -15°	-33°	-33°
SOIC_2 nd	-6°	none	-17°	-17°
Fuel Split in 1 st Injection (%)	50	none	100-0	100-0
Injection Dwell*	14°	none	16°	16°
Rail Pressure (bar)	860	860	860	600 860 1120
Inlet Boost (kPaa)	162	162	142 162 182	162
Inlet O2 (%)	21-9.5	9.5	9.5	9.5

* Injection Dwell is defined as the interval between the start of the 1st injection pulse and the start of the 2nd pulse.

Comprehensive information regarding the effects of the multiple injections can be found in the parallel research [3], however outlining of the multiple injection parameters is necessary. A convenient and descriptive way of presenting the multiple injections is one where the 1st and 2nd fuel injection timings are specified along with the percent of total fuel in the 1st injection. The reader should then be able to visualize where and when the fuel is introduced into the combustion chamber. The split-injection timings for the boost and injection pressure experiments were chosen to be -33° and -17° ATDC because of the “sweet-spot” spray targeting of the 1st injection and bowl targeting of the 2nd injection. At each experiment condition the percentages of fuel in the 1st injection were varied from 100% to 0% of the total fueling required for the constant load condition. Increments were typically 100, 90, 85, 70, 50, 30, 15, and 0%. Implicit in the fuel-split sweeps are single fuel injections at 100% and 0% with timings of the 1st and 2nd injections respectively.

Emissions data was acquired throughout all of the experiments using the Horiba emissions bench and the MKS FTIR. This allowed for many of the UHC trends to be analyzed in depth.

NUMERICAL APPROACH

COMPUTATIONAL GRID

Three dimensional computational grids with the crevice volume resolved as an elongated top land region were generated, as shown in Figure 4. To save computation load, a 1/7th sector of the full 360 degree mesh with periodic boundaries (corresponding to the seven-hole injector nozzle) was used. The average cell dimensions were 1.2~1.8 mm and 0.6~4.1 mm in radial and vertical directions, respectively. Twenty cells were generated azimuthally. To resolve the crevice region, i.e., the gap between the piston and cylinder wall above the top ring, two radial cells were used along with three vertical cells.

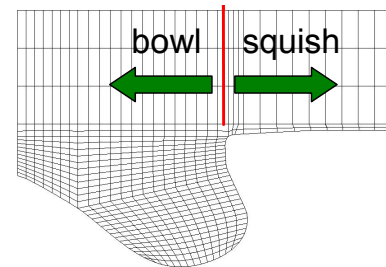


Figure 4: Vertical cross-section view of computational grid with crevice volume resolved as a thin annulus. Azimuthal angle sector span is 51.4 degrees.

SPRAY TREATMENT

Computations were performed using the KIVA3V Release 2 code [20] with an improved droplet vaporization model [21], which considers the droplet temperature range from flash-boiling conditions to normal evaporation. The improved model accounts for variable internal droplet temperature, and considers an unsteady internal heat flux with internal circulation, and a new model for the determination of the droplet surface temperature. The model uses an effective heat transfer coefficient model for the heat flux from the surrounding gas to the droplet surface. Also, the variable density of diesel fuel as a function of temperature is considered in the governing equations and the relevant sub-models.

A hybrid primary break-up model [22] that is computationally effective as well as comprehensive enough to account for the effects of aerodynamics, liquid properties and nozzle flows was employed. In this model, the injected fuel “parcels” are tracked by a Lagrangian method while the break-up of each blob is calculated from considerations of jet stability. For the secondary and further break-up processes, a Kelvin Helmholtz (KH) – Rayleigh Taylor (RT) hybrid model [22] was used.

A droplet collision model based on the stochastic particle method [20] was used, in which the collision frequency is used to calculate the probability that a drop in one parcel will undergo a collision with a drop in another parcel, assuming all drops in each parcel behave in the same manner.

The effects associated with spray/wall interactions including droplet splash, film spreading due to impingement forces, and motion due to film inertia were considered in a wall film submodel [23], in addition to calculations of film transport on complex surfaces, with heating and vaporization of the film, and separation and re-entrainment of films at sharp corners.

The RNG k- model was used for the turbulence [24] and for turbulence parameters needed in the spray model.

In the 2-phase transport equations, droplets are treated as point sources and the wall film fuel flow is not resolved on the computational grid. Therefore, it is assumed that the vaporized fuel in a computational cell where droplets or wall film parcels exist mixes completely with the gaseous mixture within the cell. Thus, stratification of gaseous species within a single cell is not resolved.

COMBUSTION TREATMENT

Detailed chemistry was employed by coupling the KIVA3V (Release 2) with the Chemkin II library [25]. A skeletal reaction mechanism for PRF fuel with 41 species and 130 reactions, which was developed by Ra and Reitz [26], was used to calculate the detailed chemical kinetics of fuel/air mixture burning.

Various mechanisms for n-heptane (or PRF0) oxidation have been widely employed for diesel combustion calculations by many researchers because of its similar ignition characteristics to those of diesel fuel. While the n-heptane mechanism [2] is used for reaction calculations in each cell, the physical properties of the fuel were represented with those of tetra-decane ($C_{14}H_{30}$) in the calculations of spray processes and in gaseous species mixing. For the calculation of NOx formation, a 4 species (N, NO, N₂O and NO₂) and 12 reaction NOx mechanism was used that has been reduced from the GRI NOx mechanism [27] and added to the PRF reaction mechanism.

A phenomenological soot model [28] modified from the Hiroyasu soot model [29] was employed to predict soot emissions. In the modified model, acetylene (C_2H_2) is used as an inception species for soot formation, which not only enables the soot model to be coupled with the detailed chemistry calculation, but also improves the soot emission predictions [28]. The soot oxidation rate

was determined by the Nagle-Strickland Constable model [30].

Recent work, as previously referenced, with this code in a number of diesel engines operating at LTC conditions indicated that it performs well predicting not only LTC ignition timing but also combustion evolution. For this reason, it was decided to apply this code to help explain the experimental results presented herein.

COMPUTATIONAL CONDITIONS

Test cases listed in the Table 6 were considered for the computations except for EGR ratio sweep. The operating conditions shown in Table 5 were used with injection timing as a parametric variable.

In Figure 5, the injection rate shape profile of a double-pulse injection is shown for the baseline injection pressure of 860 bar and a split proportion of 50 % in the first injection. The rates are normalized by the maximum value during the injection. The start of injection command of the pulses was -33° and -17° ATDC, for the first and second pulses, respectively. The duration of each pulse was 490 μ s.

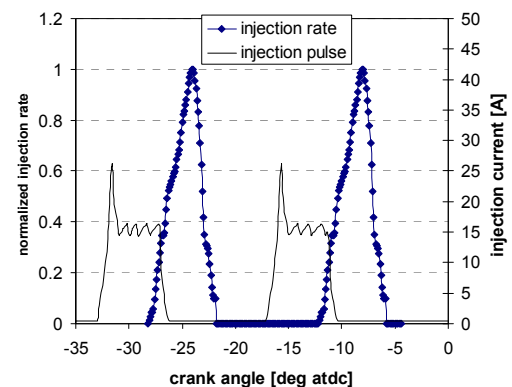


Figure 5: Measured injection rate shape of a double pulse injection. Injection pressure was 860 bar. First pulse split ratio was 50% and the duration of each pulse was 490 μ s.

PHENOMENOLOGICAL SPRAY MODEL CALCULATIONS

Calculations using a phenomenological spray model of Siewert [1] were helpful in explaining the CO “sweet-spot” observed by Kook et al. [5] and Opat et al. [6]. There, the CO increase for more advanced single-injection injection timings was linked to the amount of liquid fuel missing the piston bowl while the increase at relatively retarded timings was linked to incomplete fuel vaporization prior to SOC, thus defining a CO minimum in between. The model has been used in another study

by Siewert [31] to explain the effects of rail pressure and nozzle angle on UHC, CO, and PM emissions and thermal efficiency as affected by the computed liquid fuel missing the piston bowl during single-injection timing sweeps.

Because this current study deals with multiple injections, the situation is far more complex than the previously-mentioned single-injection studies. The model accommodates two injection events with individual spray penetration and initial droplet sizes and has been upgraded since reference [1] to calculate individual liquid lengths, vaporization times, ignition delays, and premixed and diffusion burning rates for each injection and combustion event. Both the amount of spray and liquid missing the piston bowl are now calculated automatically for each injection. Additionally, the amount of spray and liquid impinging on the bowl surfaces and bore wall each are also quantified.

The model uses a single-component fuel. For this study, fuel properties of typical diesel fuel were used, including volatility. Specifically, the volatility of tetra-decane ($C_{14}H_{30}$) was used that has a boiling point of 253°C at atmospheric pressure.

RESULTS

SOURCES OF UHC IN LTC

Initial UHC and CO emission trends and observations were presented in Figure 2. The UHC emissions do not track with the CO emissions as single injection SOIC sweeps are performed. Increased information about UHC composition was acquired using an FTIR. Future sections will discuss this information and the associated result that the total UHC can be divided into light (<6 carbon/molecule) and heavy (≥ 6 carbon/molecule) species. Currently, it is required to know of the UHC species division and that the light species can be a significant portion of the total UHC emissions.

In the boost pressure experiments outlined in Table 6, both heavy and light UHC species are reduced as increased boost pressure is implemented (shown later in Figure 24-Figure 26). By increasing the boost pressure there are globally leaner conditions. Increasing the inlet oxygen concentration also results in globally leaner conditions, and has been shown to reduce UHC emissions. To address some of the questions associated with the dominant sources of UHC emissions in LTC, the measured light UHC species (from FTIR) can be used in a chemical kinetic analysis. Homogeneous batch-reactor simulations were completed using Chemkin and a detailed n-Heptane mechanism [32]. Oxygen concentrations of 9.5% with a balance of EGR, consisting of nitrogen, CO₂, and water

vapor, were used as the initial reactor composition. The simulations were run for 2 ms at 80 bar, which is representative of the time and pressure during the main combustion event. For each simulation an equivalence ratio and a constant temperature was specified over a range of 0.01-4.0 and 500-2500K respectively. This parametric study allowed for ϕ -T maps to be generated from the batch-reactor results at the end of the 2 ms runs. Initial calculations using a UW-ERC reduced n-Heptane mechanism also showed near identical behavior to the detailed mechanism for the investigated parameters.

Figure 6 shows four predicted light UHC species formation regions from the Chemkin batch-reactor calculations. Methane, acetylene, formaldehyde, and ethylene were chosen to represent some of the light UHC species found both in the detailed n-Heptane mechanism and the experimental LTC results (discussed in the future sections). The scale on the maps was adjusted to limit the maximum value to 500 ppm of each respective species. This effectively zoomed into the maps, which would otherwise show slightly different peninsulas that behave similar to the results of Miles et al. [16]. The modified scale on the maps does not hide any behavior, but allows a closer interpretation to the actual magnitudes of UHC concentrations found in the experiments. Even though the contours were limited to 500 ppm, within that region there are certainly greater amounts of UHC species formed. This just serves as a boundary for where high regions of formation occur. Bearing in mind that these are predictions as to the chemical processes that are actually taking place; some general observations and conclusions can be inferred from them.

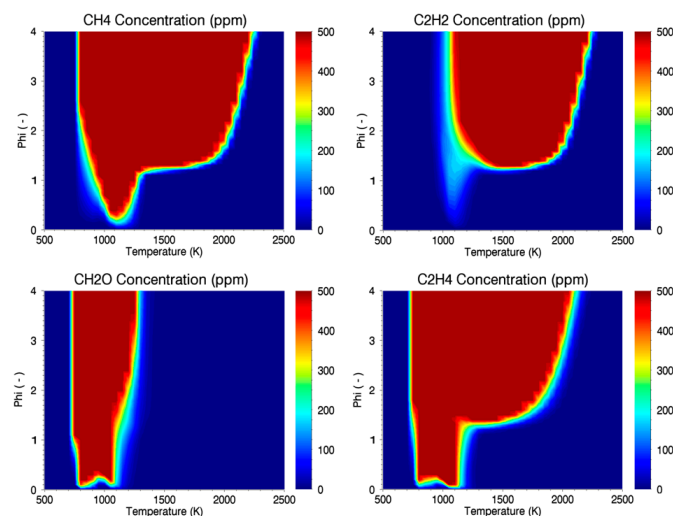


Figure 6: Homogeneous batch-reactor simulations predicting light UHC formation regions for Methane, Acetylene, Formaldehyde, and Ethylene.