On sources of CO and UHC emissions in low-temperature diesel combustion regimes

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Objectives

- **Review conventional wisdom regarding CO and UHC sources, clarifying**
  - **differences between heavy- and light-duty engines**
  - **the influence of dilution**
- **Employ the results of homogeneous reactor simulations to clarify the impact of T, ϕ, P and dilution on CO and UHC emissions**
- **Review the tools / diagnostics available to clarify dominant sources of emissions, and studies that have identified important sources under various operating conditions**

To assemble previous knowledge, fundamental underpinnings, and recent research results to provide a framework promoting clarity of thought

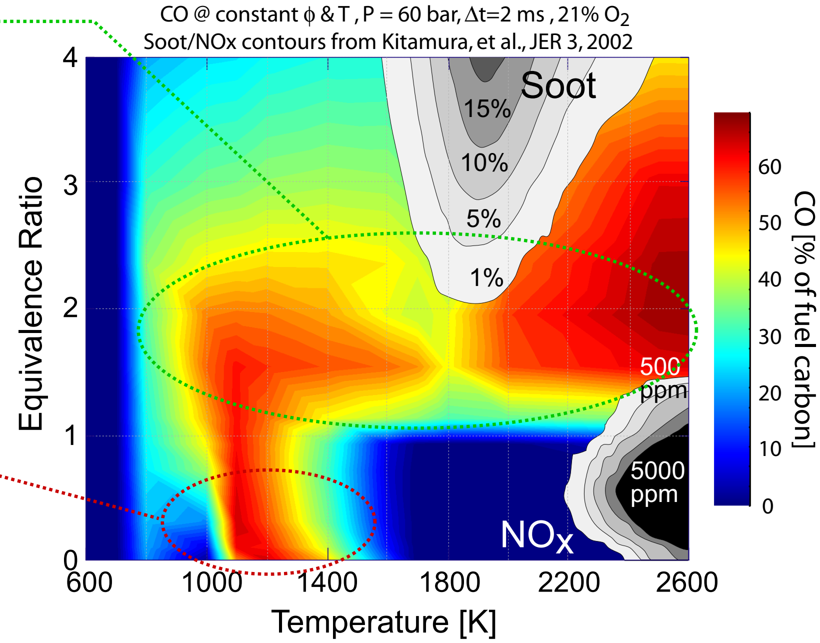
For conventional HD diesel combustion, CO emissions stem from both fuel-rich and fuel-lean regions

At high load, CO is dominated by under-mixed fuel (fuel-rich regions)

- CO tracks soot
- CO decreased with increased mixing
  - Increased P_{inj}
  - Optimized swirl

At light load, CO can be dominated by over-mixed fuel (fuel-lean regions)

- CO correlates with τ_{ig}, inversely with $T_{ad,max}$
- Can be increased with increased P_{inj}

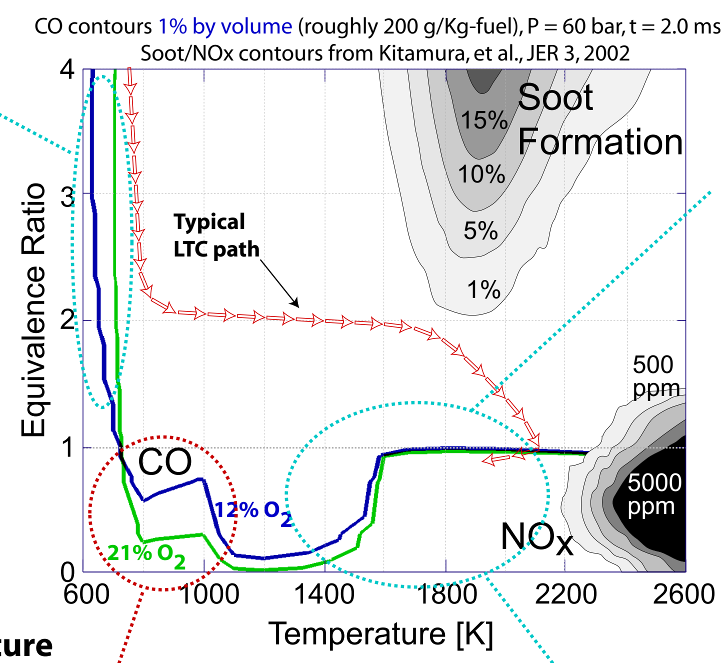


see also Park and Reitz (Comb. Sci and Tech, 2007) and Golovitchev, et al. (ICE2007) for detailed multi-dimensional calculations

With dilution, sources of CO change little

At low T, rich mixtures provide low CO: No combustion

(at a fixed, low temperature rich mixtures with EGR produce more CO)



Very little difference in oxidation behavior for T>1000 with changing dilution (EGR)

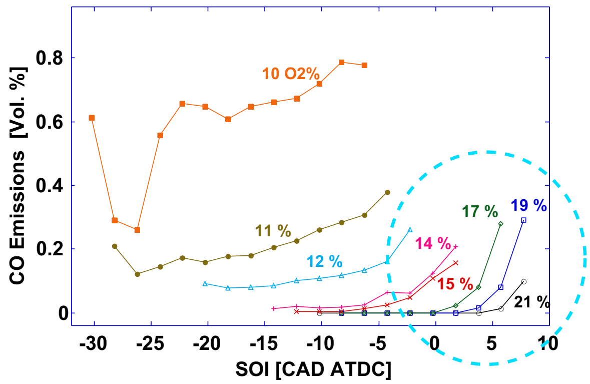
CO production in the low temperature oxidation phase is impeded by EGR (major species only)

Behavior of detailed simulations is well-captured (Park & Reitz, Golovitchev et al.)

Conclusion:

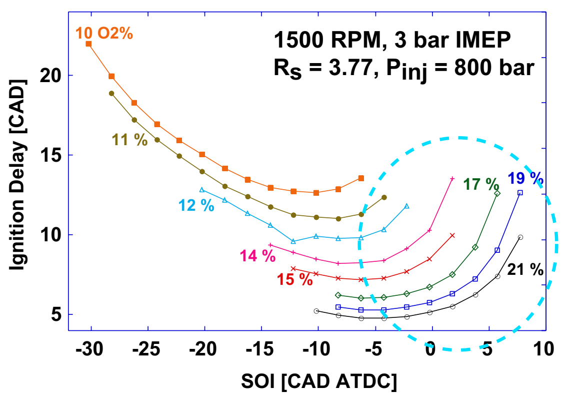
Fuel mixed with sufficient O_2, early enough to allow 2 ms at T>1600K, will burn completely

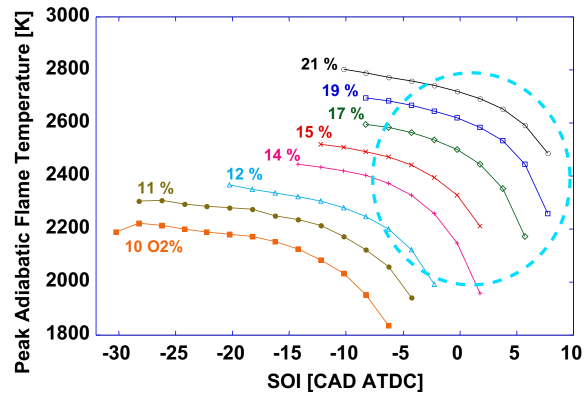
At light load, moderate EGR, and retarded SOI (MK-like), CO stems from over-mixed fuel (lean mixtures)



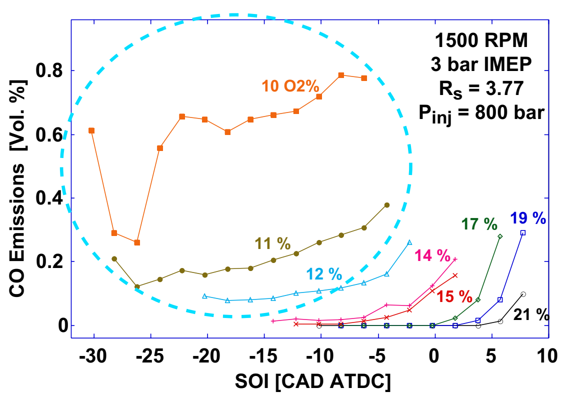
Increased CO correlates well with increased ignition delay and with decreasing peak flame temperature

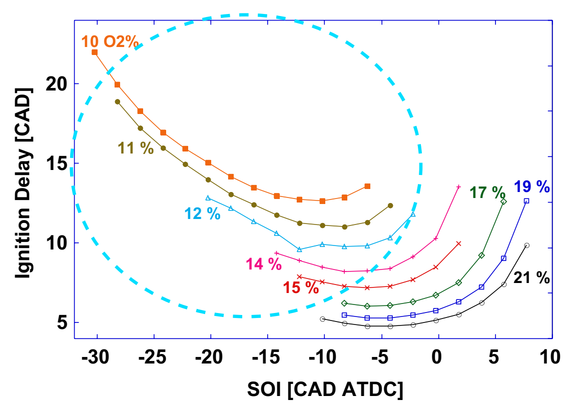
Modeling studies employing quasi-detailed kinetics show engine-out CO comes from over-lean regions
(Adomeit, et al, THIESEL 2004)



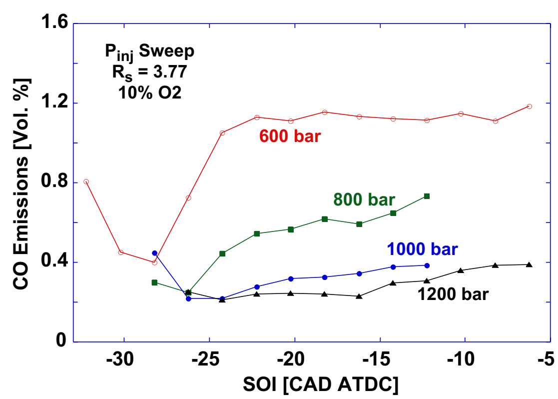


With high-dilution, CO emissions are dominated by under-mixed fuel





- **At high EGR rates increased CO emissions correlate inversely with ignition delay**
- **We also generally observe a sharp decrease in CO emission with increased injection pressure (note early SOI behavior)**

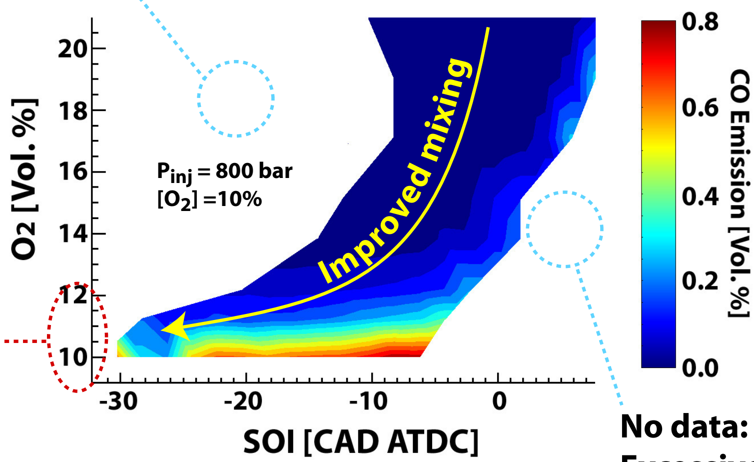


CO emissions increase with EGR, but can be improved by enhancing mixing

No data: Excessive $\frac{dP}{d\theta}$

Advancing SOI increases mixing time (and effectiveness)...

... leading to acceptable CO emissions (up to a point)



CO emissions *increase* as SOI is further advanced

No data: Excessive ISFC

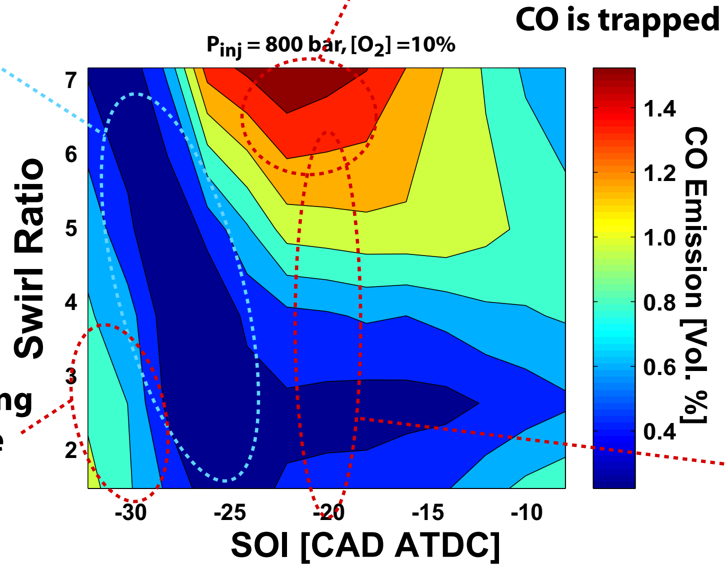
What aspect of mixing is influenced? Time or effectiveness? Early or late?

Mixing can be improved (or worsened) by changing swirl or injection timing

Due to enhanced early mixing

- Experimental heat release analysis
- Numerical simulations

Very high CO emissions are observed at high swirl ratio. CO is trapped in the bowl



SAE 2006-01-0197

Optimal swirl ratio due to bulk flow structures that enhance late mixing

Piston top wetting and/or excessive squish volume penetration impedes mixing (less so at high swirl, more so at high injection pressure)

Similar behavior observed in a GM 1.9 liter engine by Opat, et al. (see SAE 2007-01-0193)

CO emissions can also be reduced by increasing boost

When CO emissions are dominated by under-mixed fuel:

1) The global equivalence ratio decreases

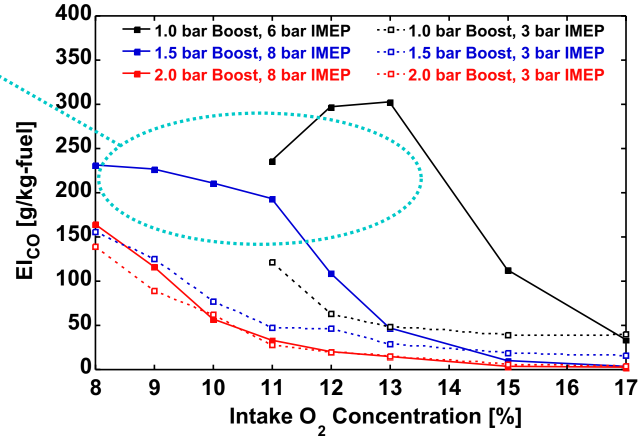
2) Mixing is more rapid

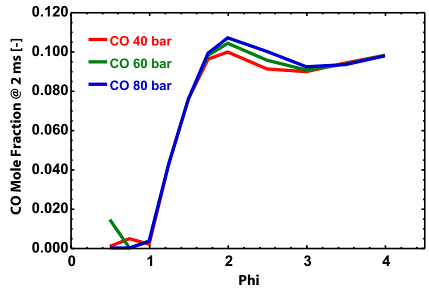
- For free jets: $\frac{d\phi}{dt} \sim \rho^{0.25}$

- In engines: B70-90 $\sim \rho^{-1}$

3) Changes in kinetics with boost are relatively unimportant $\Rightarrow$

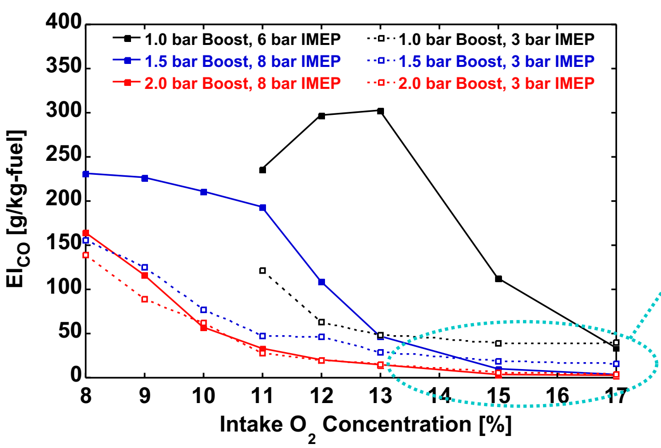
Emissions from a GM automotive diesel at 1500 rpm
(see also Noehre, et al., SAE 2006-01-3412, for HD engines





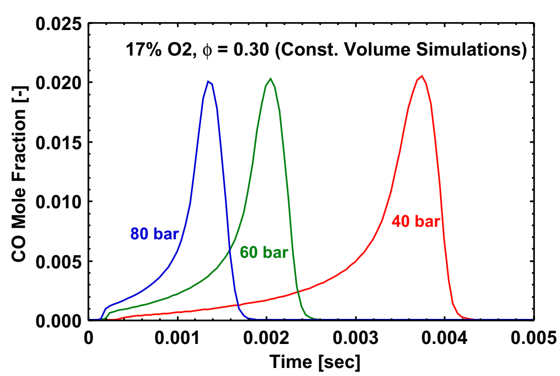
For rich mixtures, CO formation is rapid and levels determined by available O_2

CO emissions stemming from lean mixtures can also benefit from boost



When CO is dominated by over-mixed fuel, boost helps by speeding reaction

$\Downarrow$



Careful interpreting CO contours...

- Constant T, P simulations don't allow heat generated from combustion to speed reaction)
- CO yield at 2 ms is higher at 60 bar than 40, yet combustion is considerably faster

CO summary

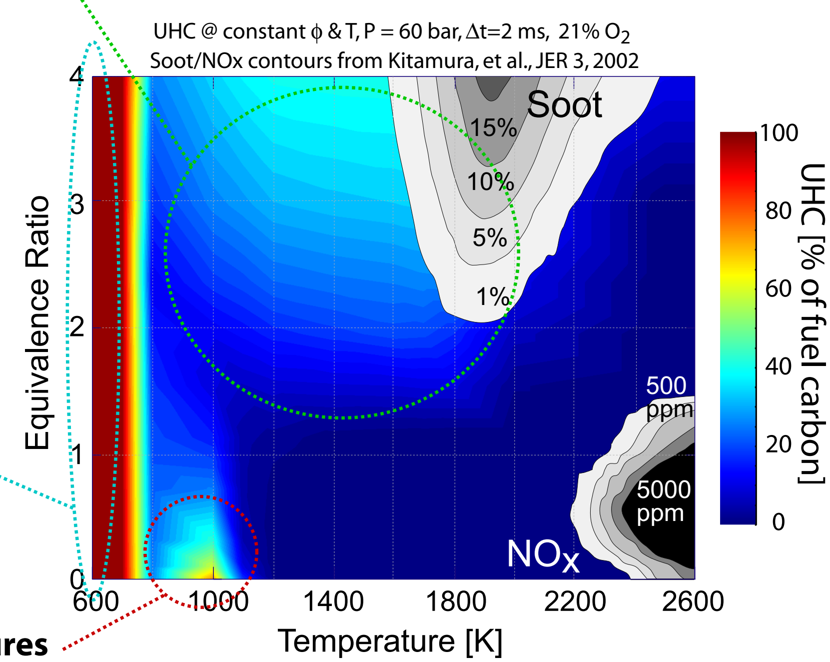
Like conventional diesel combustion, CO emissions from low-temperature combustion systems can be dominated by either rich pockets (under-mixed fuel) or by lean pockets (over-mixed fuel) depending on load, EGR rate, SOI, etc.

- **When under-mixed fuel dominates CO emissions, emissions can be reduced by**
  - **Increased injection pressure** (see also MTZ Sept 2003, 2007-01-0193)
  - **Appropriate injection timing/targeting**
  - **Formation of beneficial late-cycle flow structures**
  - **Increasing boost (both λ and ρ are increased)**
- **When over-mixed fuel dominates CO emissions, emissions can be reduced by**
  - **Increasing boost (can significantly speed reaction rates)**
  - **Reducing P_{inj}** (2006-01-0076, ...)

For conventional HD diesel combustion, UHC is known to stem from low temperature and fuel-lean regions

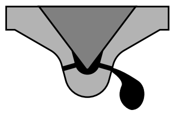
Poor mixture formation
- Low injection velocity
- Large droplets (may delay mixing)
- Under- or over-penetration

Cold quench layers on combustion chamber walls

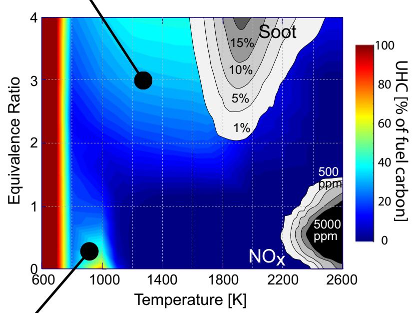


Over-lean mixtures (formed during τ_{ig})

For well-optimized HD engines, two UHC sources are generally thought to dominate



Sac volume / hole dribble



Lean mixtures formed during ignition delay

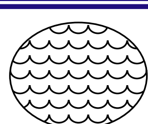
Conventional strategies to reduce UHC:

- ⊘ **Reduce sac volume**
- ⊘ **Micro-holes - Not!** (SAE 2005-01-0914)
- ⊘ **Decrease τ_{ig}**
  - Increase compression ratio
  - Increase coolant temperature
  - Increase T_{intake}
  - Increase displacement
- **Optimize mixing**
  - Nozzle hole number
  - Nozzle hole area
  - Swirl
  - Bowl design
- **Increase boost**
- **Increase cetane number**

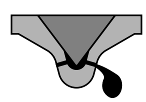
⊘ Undesirable for LTC or high power density applications

For light-duty engines, additional UHC sources become important

Liquid films



- Survive multiple engine cycles
- Delay vaporization and mixing

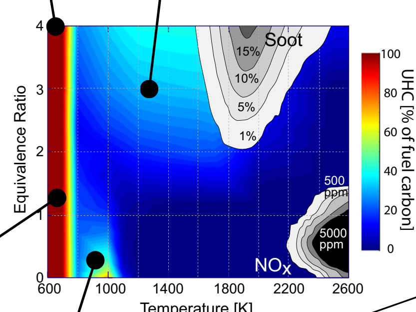


Increased importance due to smaller displacement

Complete mixing more difficult due to lower global λ (high power density)

Squish-volume quench layers

- More significant for high-squish, re-entrant bowls



Lean mixtures remain important at light load

Additional strategies to reduce light-duty UHC:

- **Increase bowl diameter**
- **Disrupt film formation** (may impact high-load performance)
- **Post-injection** (not well understood)
- **Close pilot injections**
- **Reduce spray asymmetry**
- **Optimize mixing** (swirl, bowl design, targeting)

What happens when we add significant EGR?

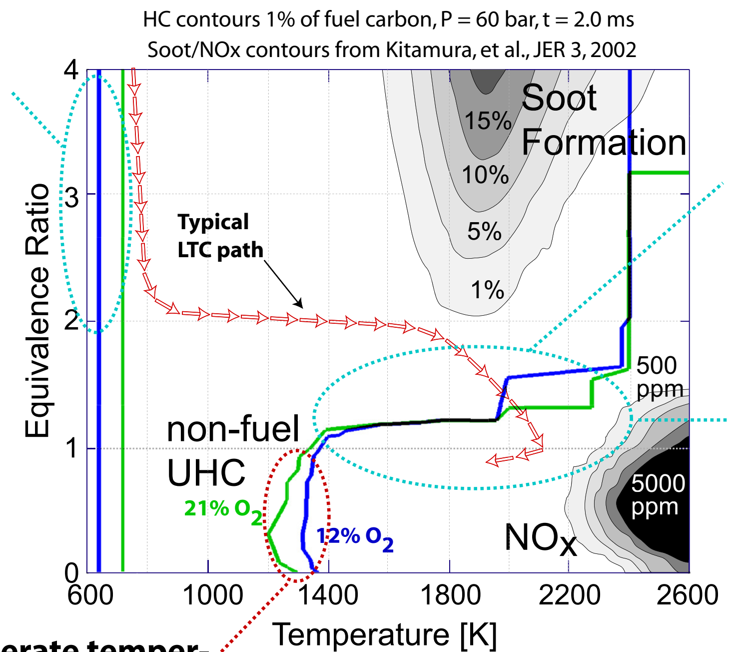
Like CO, UHC yield is not strongly influenced by dilution

EGR promotes low temperature formation of non-fuel UHC

- Enhanced CO production, too

EGR may reduce UHC emissions

- "re-burning" recirculated UHC
- Enhanced low temperature oxidation (see also JSAE 20030230)



Low HC yield is observed from moderately rich mixtures

In the region of most interest, EGR has little influence

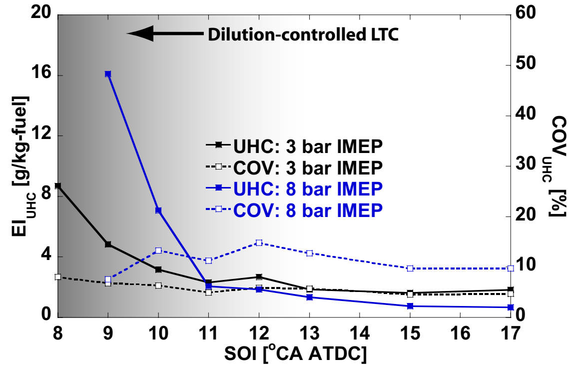
(a small advantage to EGR is seen at the higher T, ϕ)

For ϕ<1 and moderate temperature, EGR inhibits HC oxidation

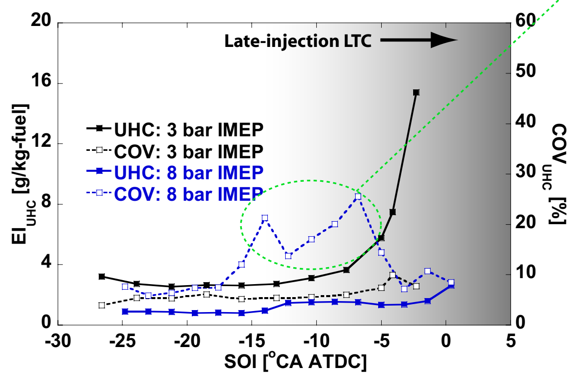
Tools available to identify UHC sources

- **Cycle-resolved UHC measurements obtained via fast FID**
- **Load / parameter sweeps to identify controlling processes**
- **Optical measurements**
  - Liquid film imaging
  - Imaging of in-cylinder UHC distributions
- **Modeling predictions**
  - Homogeneous reactors
  - Multi-dimensional simulations using detailed kinetics
  - Liquid impingement calculations
- **UHC emission behavior contrasted with CO emissions**
- **Speciated UHC measurements**
- **Fuel effects**

Fast-FID measurements indicate that the COV of UHC emissions remains small even while mean emissions rise



Dilution Controlled LTC



Late-Injection LTC

Both low-load and moderate-load UHC emissions, for both dilution-controlled and late-injection low temperature combustion systems, exhibit low cycle-to-cycle COV.

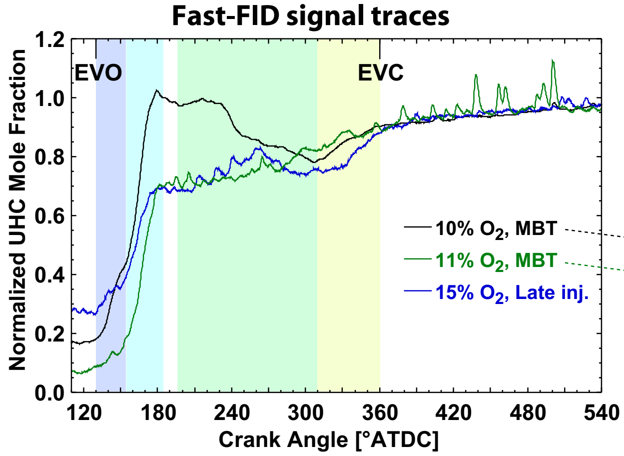
(anomalous spikes in single cycles occasionally give the appearance of high COV)

Conclusion:

Multiple-cycle combustion modeling / optimization will not be required to design of optimal UHC emissions. The physics responsible for increased UHC should be captured in the "mean" cycle

Fast FID measurements can provide useful information on sources and spatial distributions of UHC

Fast-FID signal traces



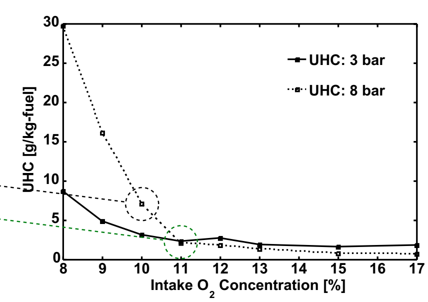
Head/valve crevices, sac dribble

Initial blowdown - upper cylinder

Exhaust stroke - lower cylinder

Cylinder wall, piston top, bowl layers

Why do UHC emissions increase with increased dilution?



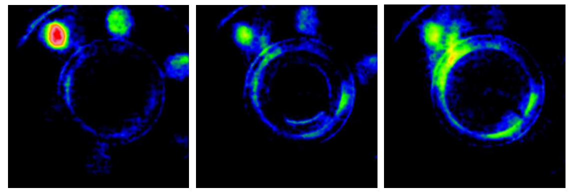
- **Proportionately more UHC stems from the upper portion of the cylinder at lower [O_2], consistent with earlier SOI required for MBT** (Load behavior suggests this is due to rich regions)
- **Higher [O_2] conditions (including late injection) show greater UHC from lower in the cylinder**

(Kinetics limited, thermal gradients?)

Liquid films clearly form in DI diesel engines with early injection, and can survive well into the exhaust stroke

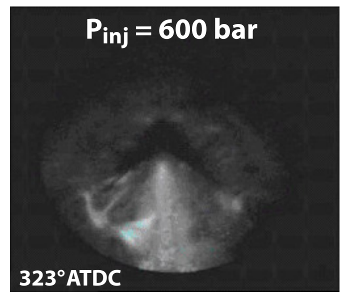
Spray footprints on the piston top can be observed directly for early SOI

Fuel films detected via LIF rapidly lose definition after EVO – behavior consistent with flash boiling



Fuel clouds imaged during the exhaust stroke support this interpretation

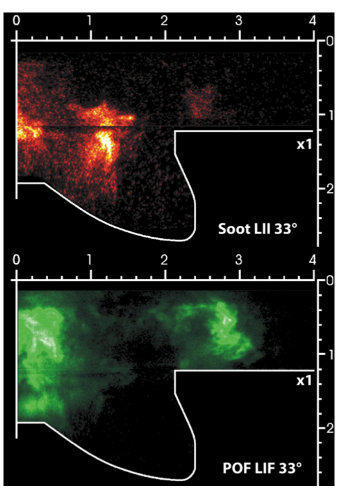
(Images and analysis courtesy of Julian Kashdan, IFP JSAE 20077038)



Accurate representation of real engine film behavior is difficult

- Optical piston temperatures can differ significantly from metal pistons
- Skip-firing can lead to atypical behavior (film lifetimes may be several engine cycles when continuously fired)

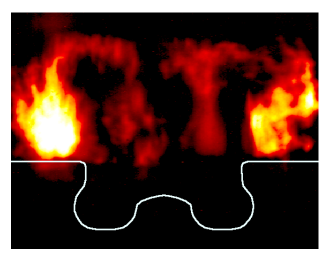
UHC (and soot) in early-injection PCI combustion systems are indicative of rich-region "bulk gas" UHC sources



Non-selective LIF of partially-oxidized fuel in a Volvo D5 for dilute (12% O2) LT combustion

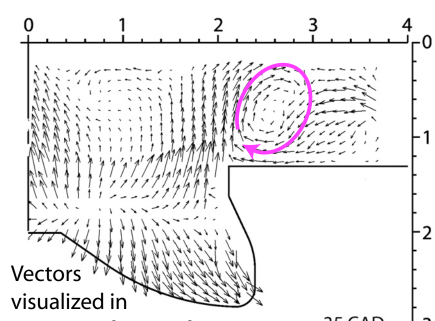
Soot and/or partially-oxidized fuel is located just above the piston top during the expansion stroke

Similar distributions of soot have been seen for conventional diesel combustion

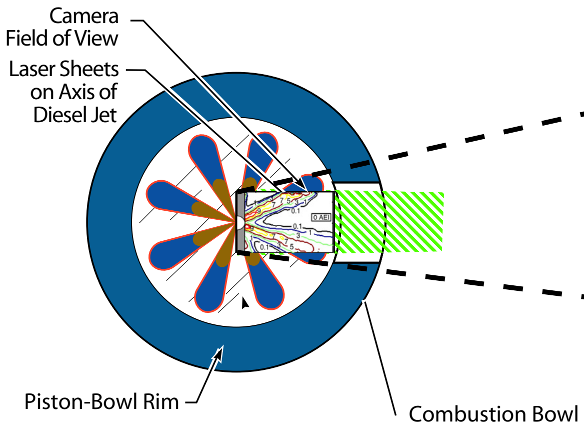


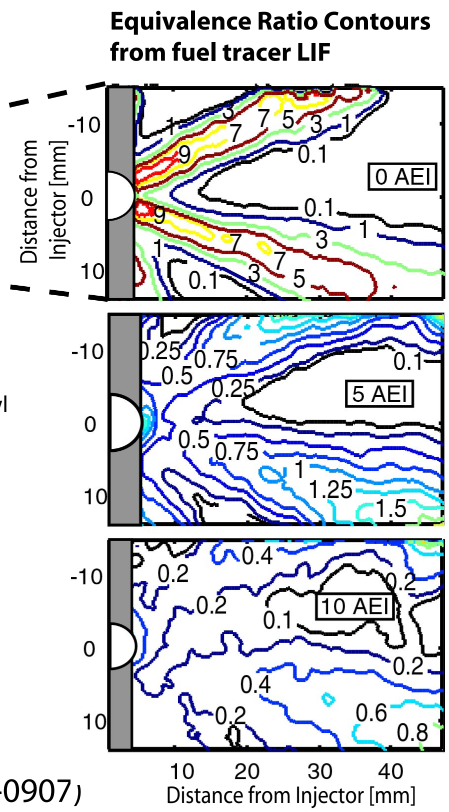
Soot distributions observed for conventional diesel combustion

Flow measurements show that mixing is impeded by a toroidal vortex situated above the piston top ... Can this vortex be disrupted?



For positive ignition dwell LTC, lean mixtures formed after EOI may be an important source of UHC



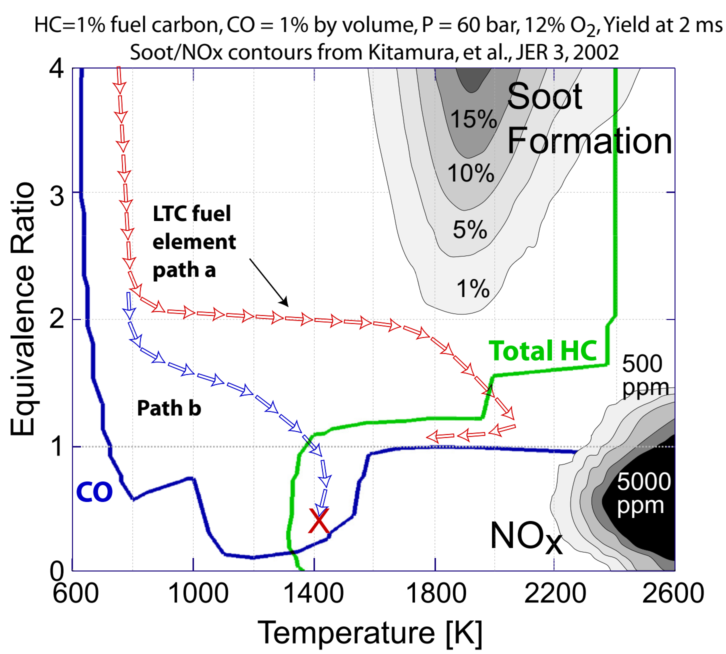


Cummins N-14, 2.3ℓ HD engine
4 bar IMEP fuel load, 12.7% O_2

- **Fuel air equivalence ratios rapidly become lean in the trailing portion of the jet**
- **Imaging of CH_2O indicates that partially-burned fuel from this region persists well into expansion**

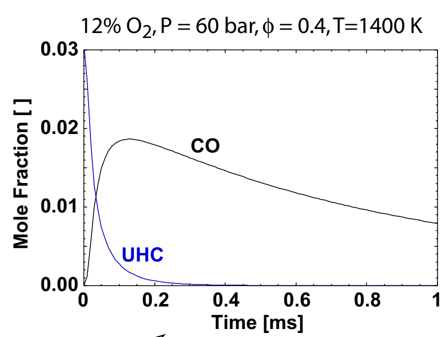
(Data/Analysis from Musculus, et al. SAE 2007-01-0907)

Homogeneous reactor modeling studies help identify situations which result in high CO but low HC



a) Combustion near λ=1 (high load or EGR rate)

- Even with high late-cycle mixing rates, there may be insufficient O2 available locally to achieve mixtures with $\phi < 1$



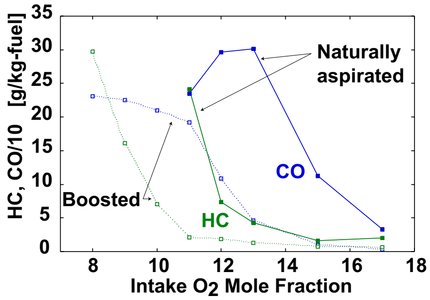
b) Quenching of lean mixtures during expansion

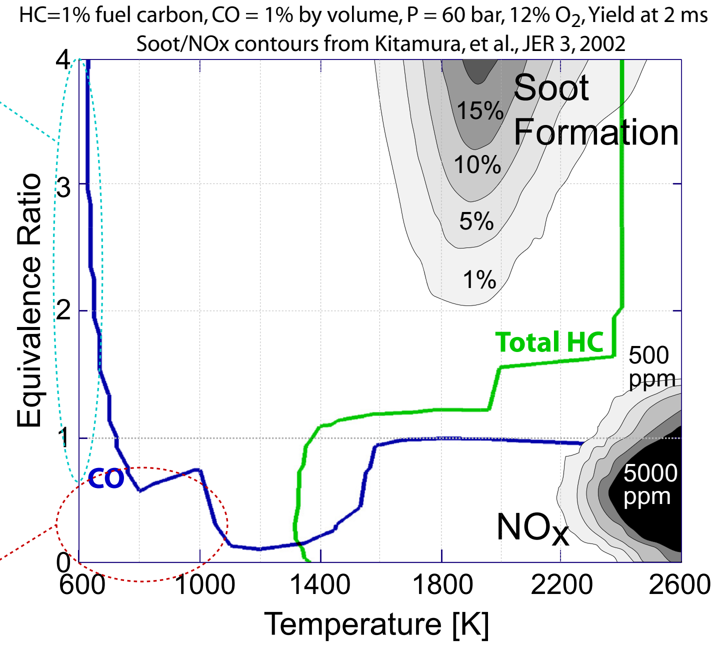
- HCs can be consumed well before CO oxidation is complete

Conversely, high HC but low CO may be observed

Cold crevices regions can result in high HC with very little CO…

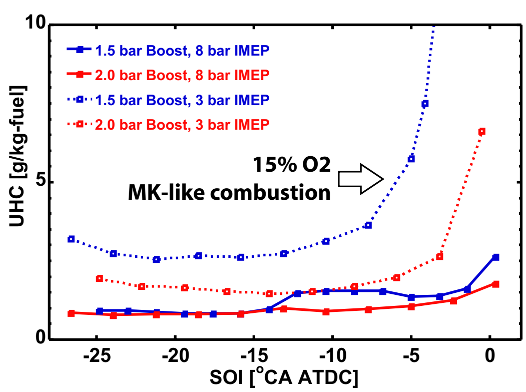
…so can liquid films!

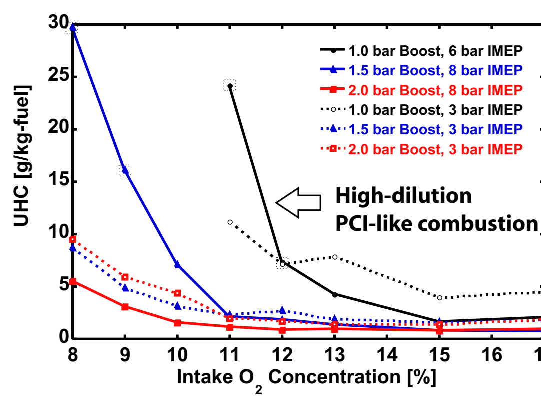




Cool–moderate temperature lean regions can also lead to HC emissions with little CO

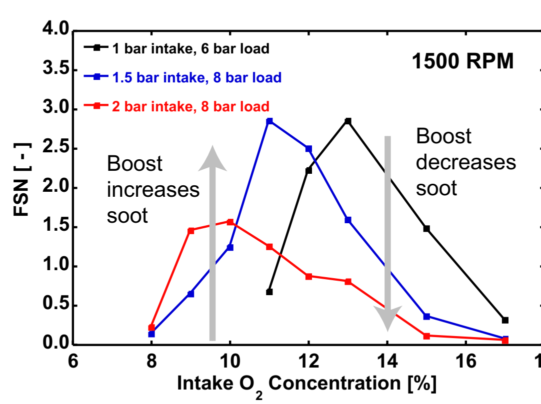
Like CO, UHC emissions can be reduced over a wide spectrum of operating conditions with increased boost



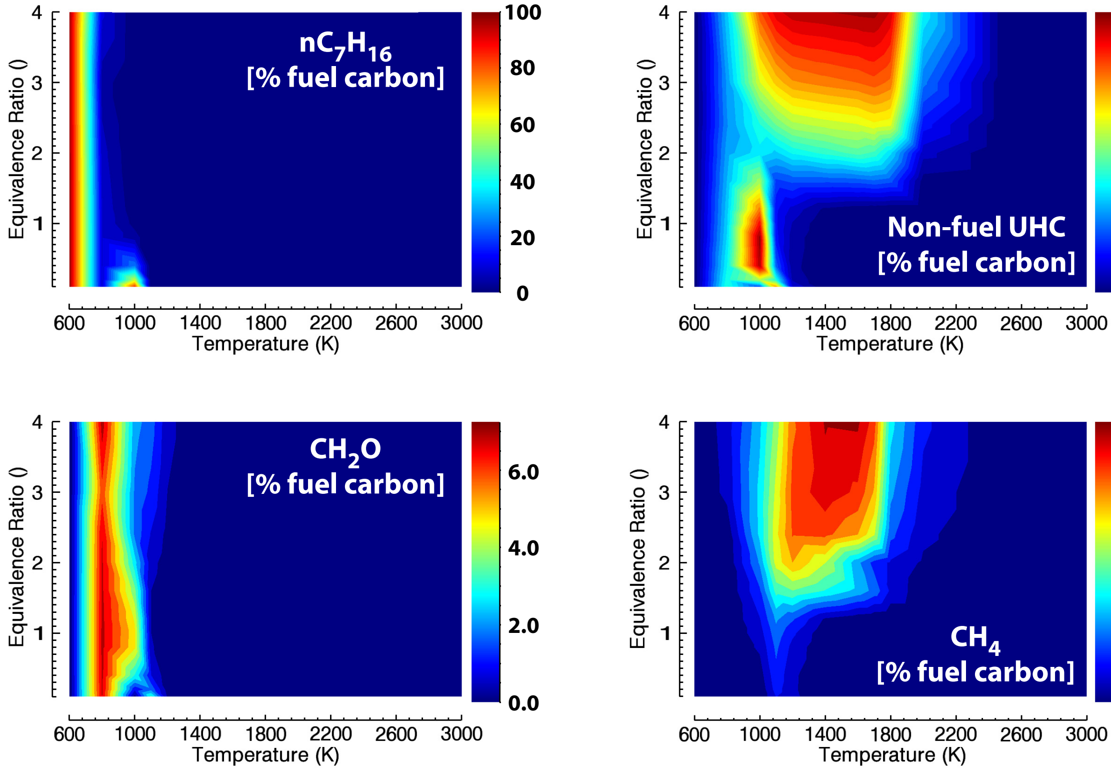


Boost is not uniformly beneficial!

Soot can be increased significantly at low O_2 and high manifold pressures



Speciation of HC emissions can provide information on the sources of UHC



UHC summary

- Like CO emissions, UHC can stem from either rich pockets (under-mixed fuel) or by lean pockets (over-mixed fuel). Direct in-cylinder imaging studies have shown either source can dominate, depending on conditions
- Unlike CO, UHC emissions can also stem from cold boundary layer or crevice regions. This source may also dominate under some conditions.
- Homogeneous reactor simulations suggest that dilution has only a small effect on UHC emissions at a fixed T and ϕ.
- EGR may reduce UHC emissions stemming from cold regions (at the expense of increased CO emissions)
- Boost increases both chemical rates and mixing rates, and can reduce UHC stemming from over-lean and over-rich regions (Careful! There may be a soot penalty)

Closure

- There is no simple answer to the question "What is the dominant source of UHC in low-temperature diesel combustion systems. Under-mixed fuel, over-mixed fuel, and crevice/wall layers can all play important roles
- Understanding and controlling the mixture formation process including
  - Sufficiently rapid mixing of fuel-rich regions
  - Avoidance of over-mixing
  - Avoidance of HC in crevices and quench layers
  - Avoidance of liquid films

  is key to the successful development of low-temperature diesel combustion systems