Sources and mitigation of CO and UHC emissions in low-temperature diesel combustion regimes: Insights obtained via homogeneous reactor modeling

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Objectives

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

- **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 summarize studies that have identified important sources under various operating conditions**

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

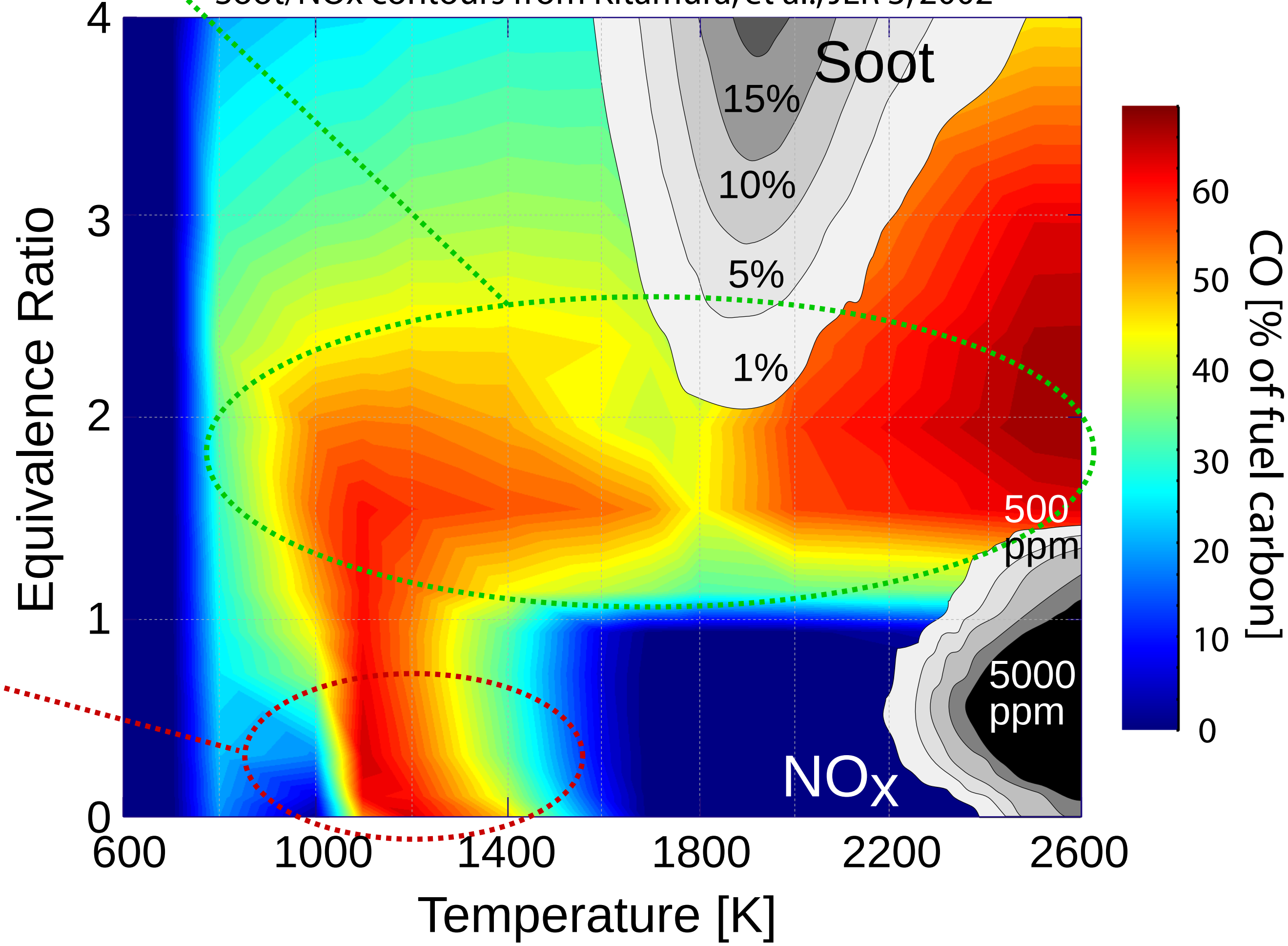
At high load, CO is dominated by under-mixed fuel (fuel-rich regions)

- 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}

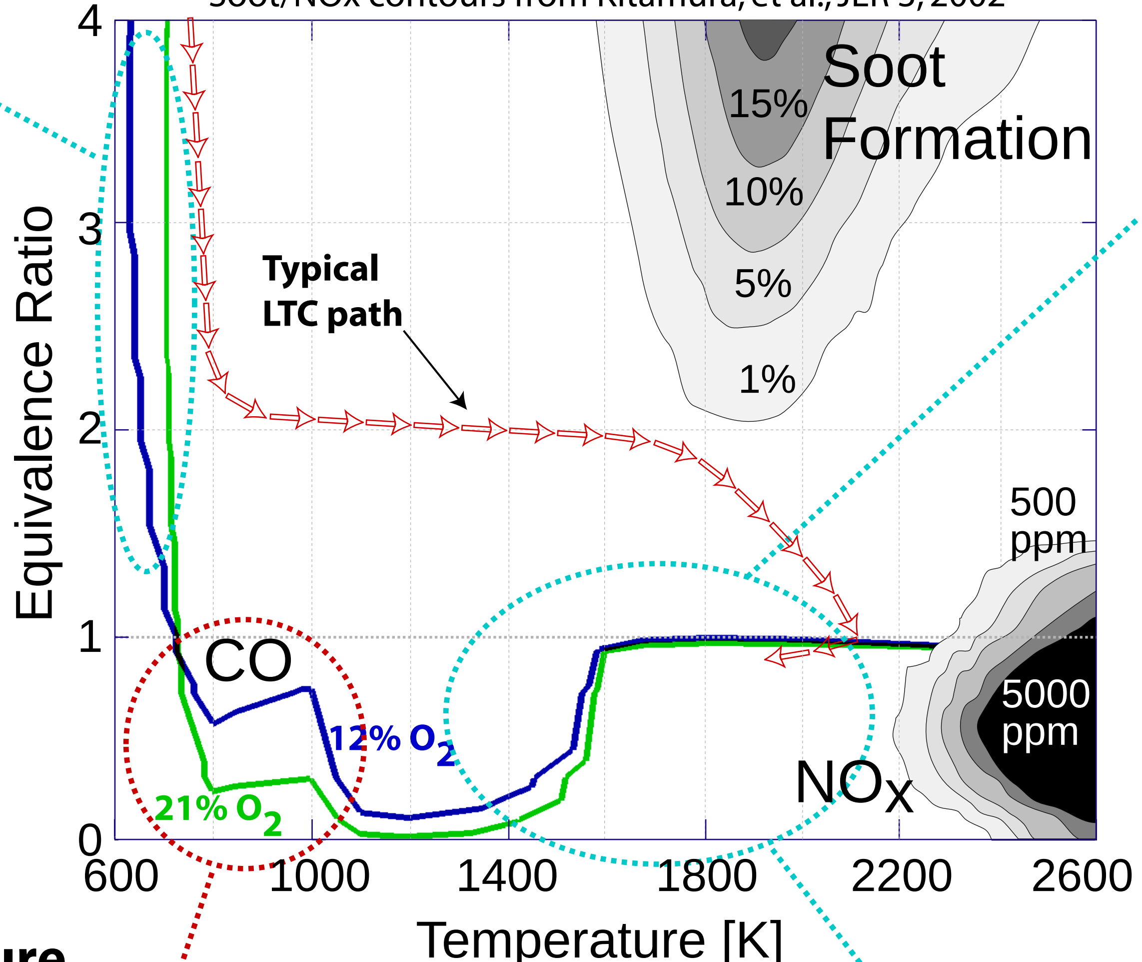
CO @ constant ϕ & T , P = 60 bar, Δt=2 ms , 21% O_2
Soot/NOx contours from Kitamura, et al., JER 3, 2002



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

CO contours 1% by volume (roughly 200 g/Kg-fuel), P = 60 bar, t = 2.0 ms
Soot/NOx contours from Kitamura, et al., JER 3, 2002



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

CO – Summary of recent LTC studies

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. (2005-01-3837, 2006-01-0197, 2007-01-0193)

- **When under-mixed fuel dominates CO emissions, emissions can be reduced by**
  - **Increased injection pressure** (see also MTZ Sept 2003)
  - **Appropriate injection timing/targeting**
  - **Formation of beneficial late-cycle flow structures**
  - **Increasing boost (both λ and ρ are increased)** (see also 2006-01-3412, Colban, et al. SAE 2008)
- **When over-mixed fuel dominates CO emissions, emissions can be reduced by**
  - **Increasing boost (increased reaction rates dominate)**
  - **Reducing P_{inj}** (2006-01-0076)

Dilution has little influence on the completion of CO oxidation

Potential UHC sources include poorly mixed, fuel-rich regions, fuel-lean regions, and low temperature regions

Poor mixture formation

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

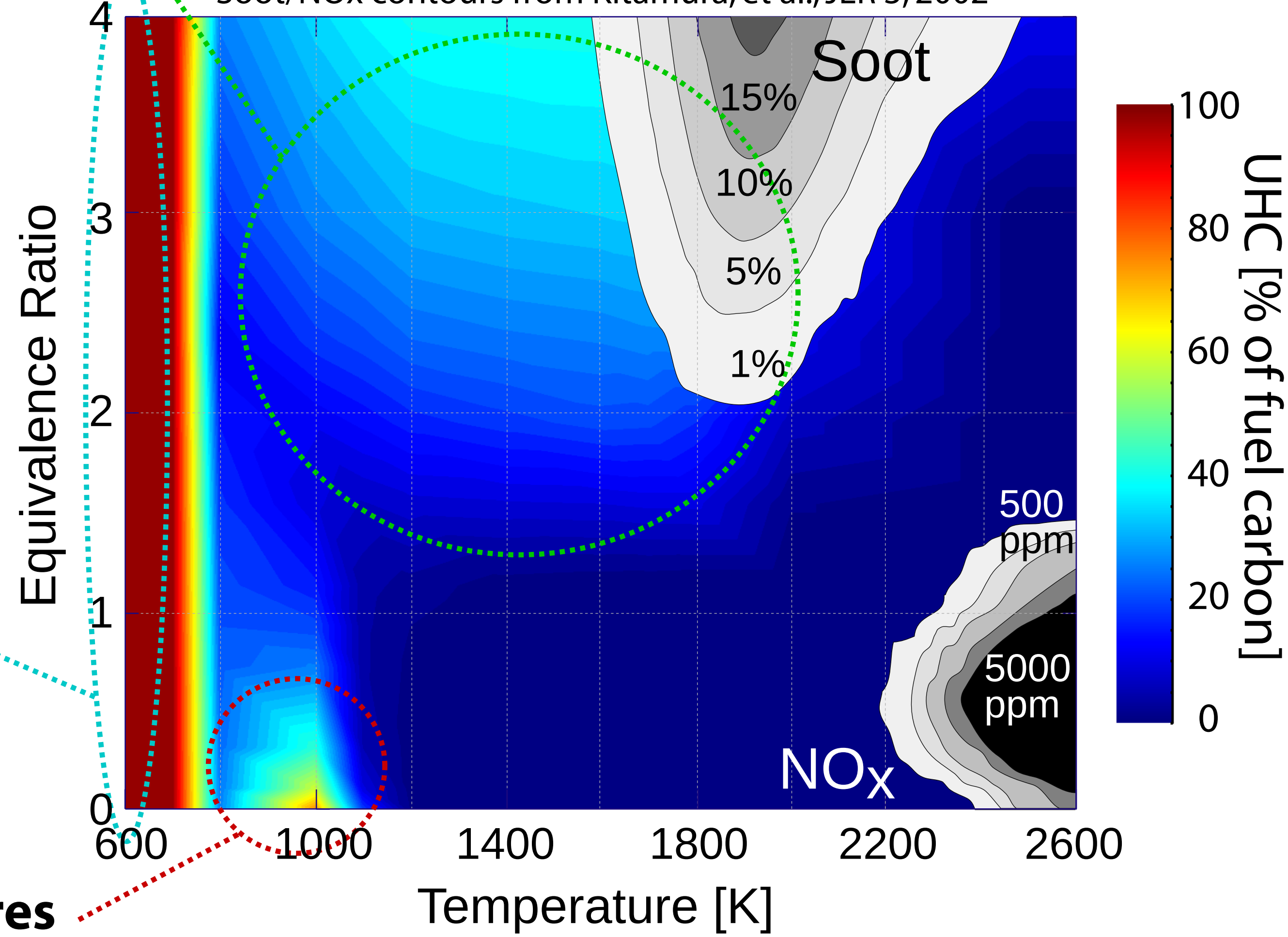
(e.g. Greeves, Khan, etc.)

Cold quench layers on combustion chamber walls

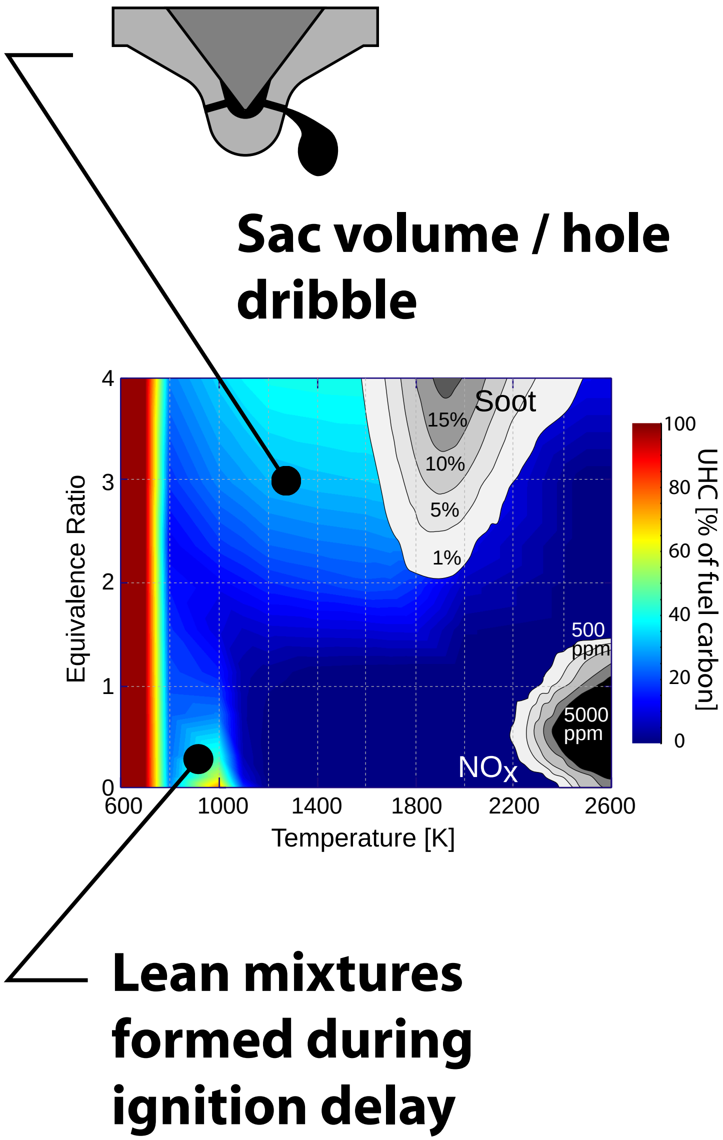
Over-lean mixtures

(formed during τ_{ig})

UHC @ constant ϕ & T, P = 60 bar, Δt=2 ms, 21% O_2
Soot/NOx contours from Kitamura, et al., JER 3, 2002



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



Conventional strategies to reduce UHC:

Reduce sac volume

Decrease τ_{ig}
- Increase compression ratio
- Increase coolant temperature
- Increase T_{intake}
- Increase displacement

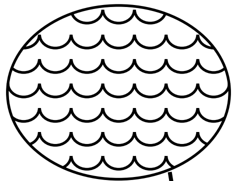
Optimize mixing
- Nozzle hole number
- Nozzle hole area
- Swirl
- Bowl design
- Micro-holes - Not! (SAE 2005-01-0914)

Increase boost

Increase cetane number (SAE 2004-01-1868)

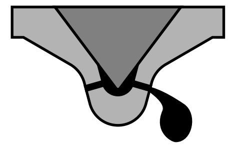
Undesirable for LTC or high power density applications

For light-duty engines, additional UHC sources become important



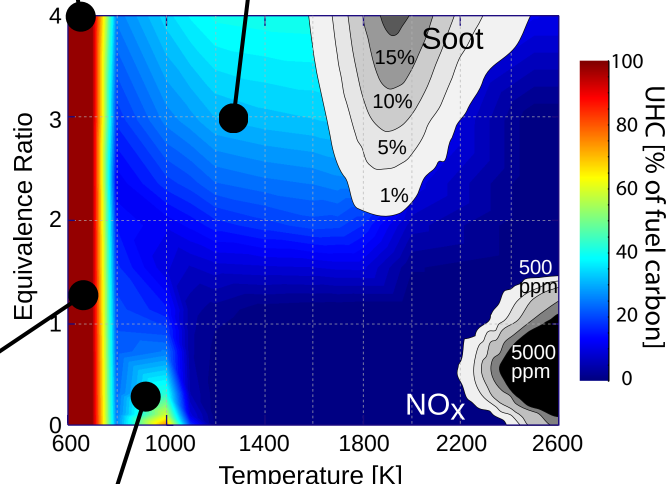
Liquid films

- 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

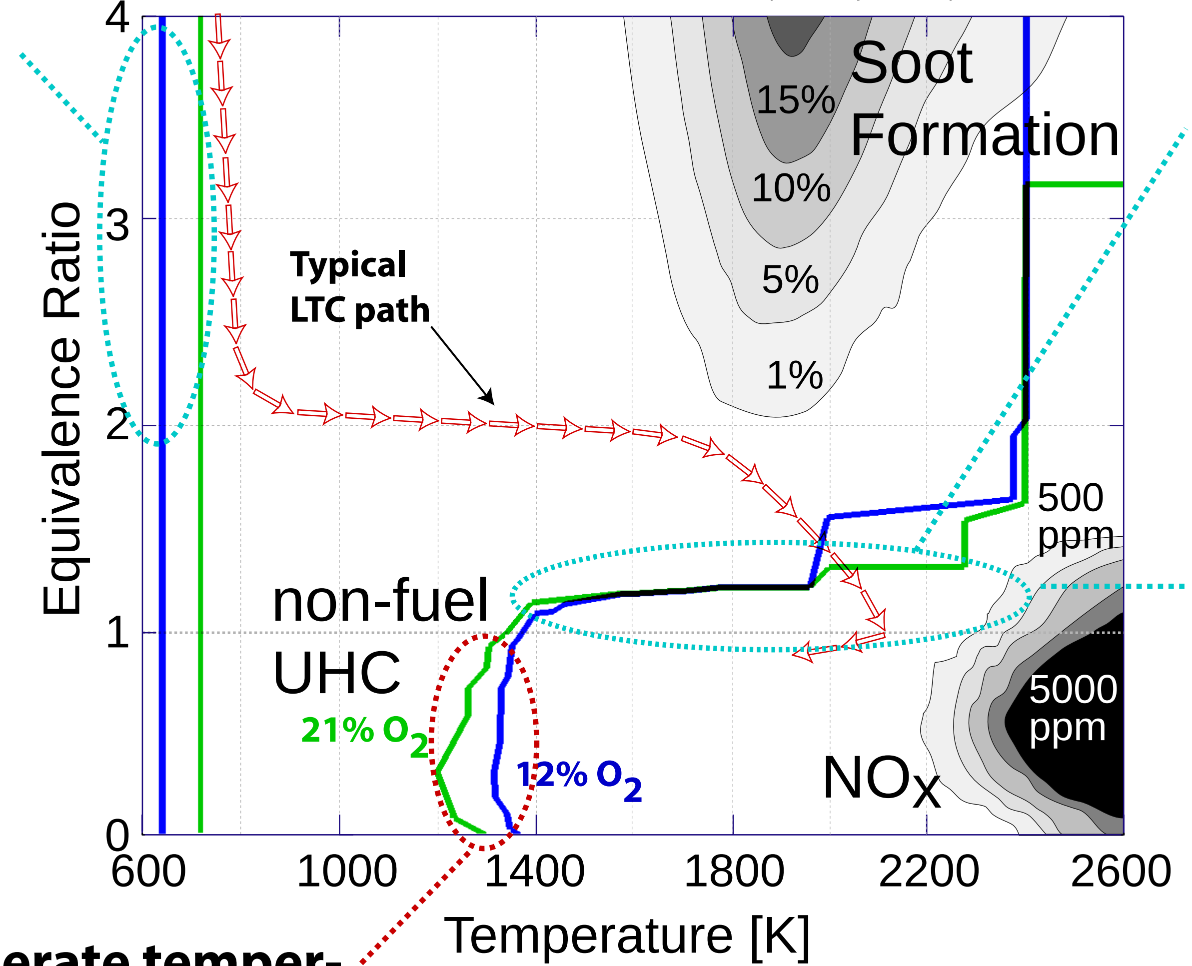
EGR promotes low temperature formation of non-fuel UHC

- Enhanced CO production, too

EGR may reduce UHC emissions

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

HC contours 1% of fuel carbon, P = 60 bar, t = 2.0 ms
Soot/NOx contours from Kitamura, et al., JER 3, 2002



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)

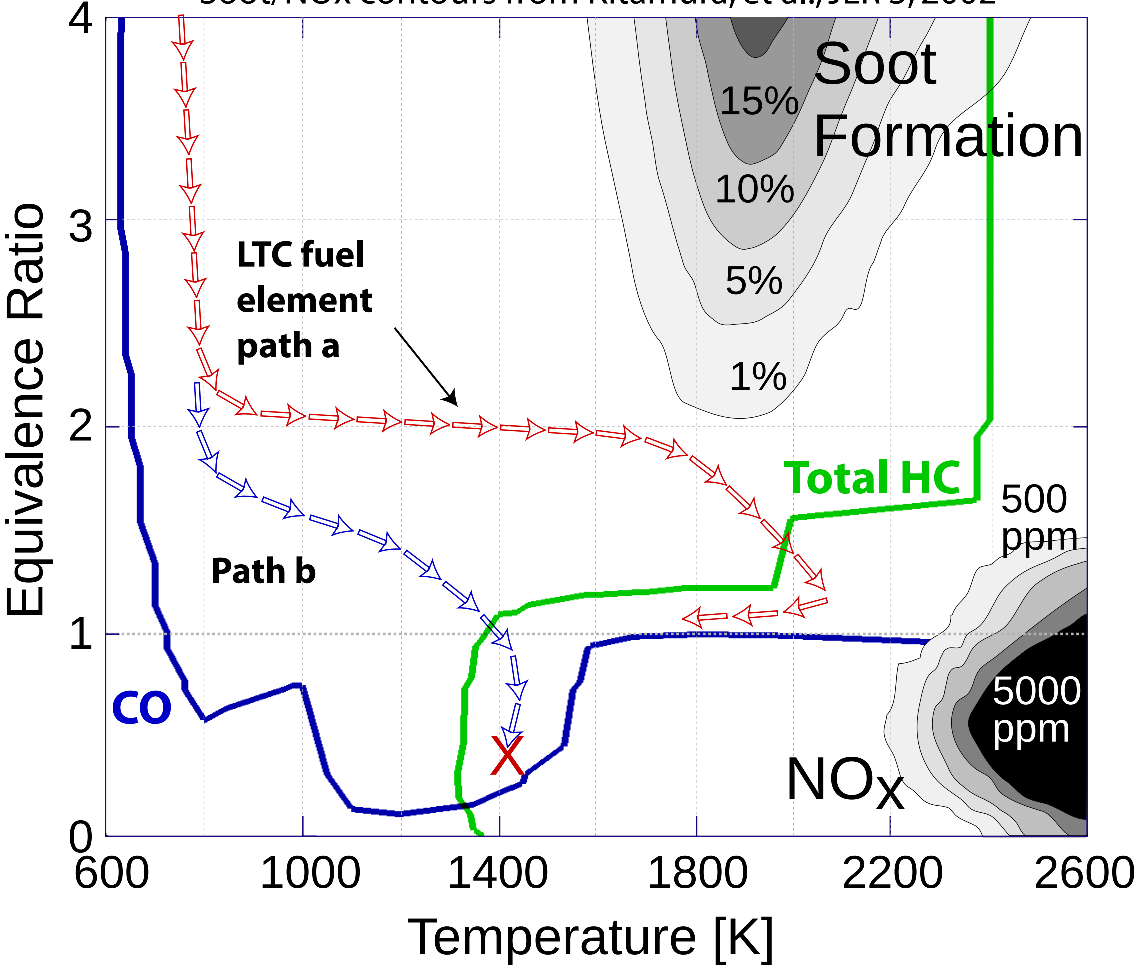
For ϕ<1 and moderate temperature, EGR inhibits HC oxidation

Tools available to identify UHC sources

- **Cycle-resolved UHC measurements obtained via fast FID** (2007-01-1837)
- **Load / parameter sweeps to identify controlling processes**
- **Optical measurements**
  - Liquid film imaging (2007-01-1836)
  - Imaging of in-cylinder UHC (2007-01-0907; Proc. Comb Inst. 31, 2963-2970)
- **Modeling predictions**
  - Homogeneous reactors
  - Multi-dimensional simulations using detailed kinetics (Park & Reitz, CST 2007)
  - Liquid impingement calculations
- **UHC emission behavior contrasted with CO emissions**
- **Speciated UHC measurements**
- **Fuel effects**

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

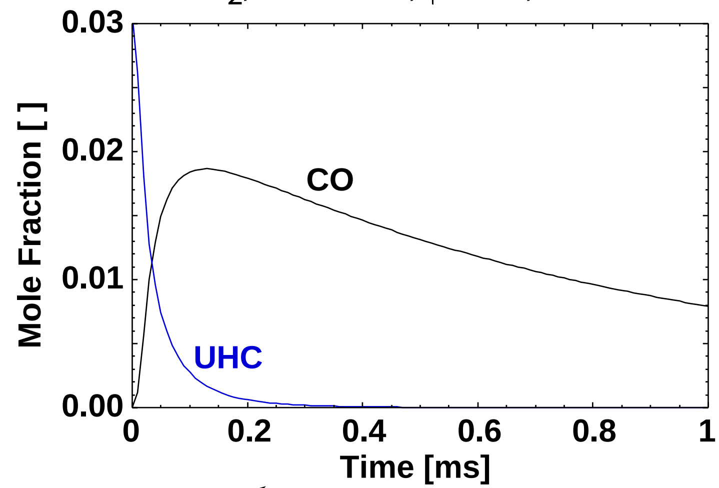
HC=1% fuel carbon, CO = 1% by volume, P = 60 bar, 12% O_2, Yield at 2 ms
Soot/NOx contours from Kitamura, et al., JER 3, 2002



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 $\phi < 1$

12% O_2, P = 60 bar, ϕ = 0.4, T=1400 K



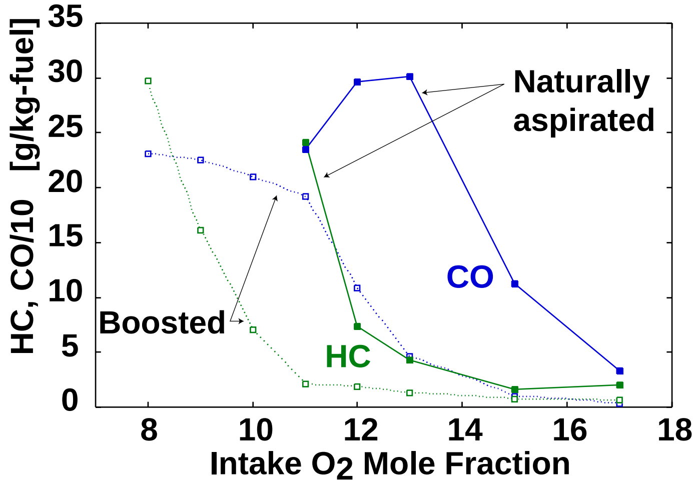
b) Quenching of lean mixtures during expansion

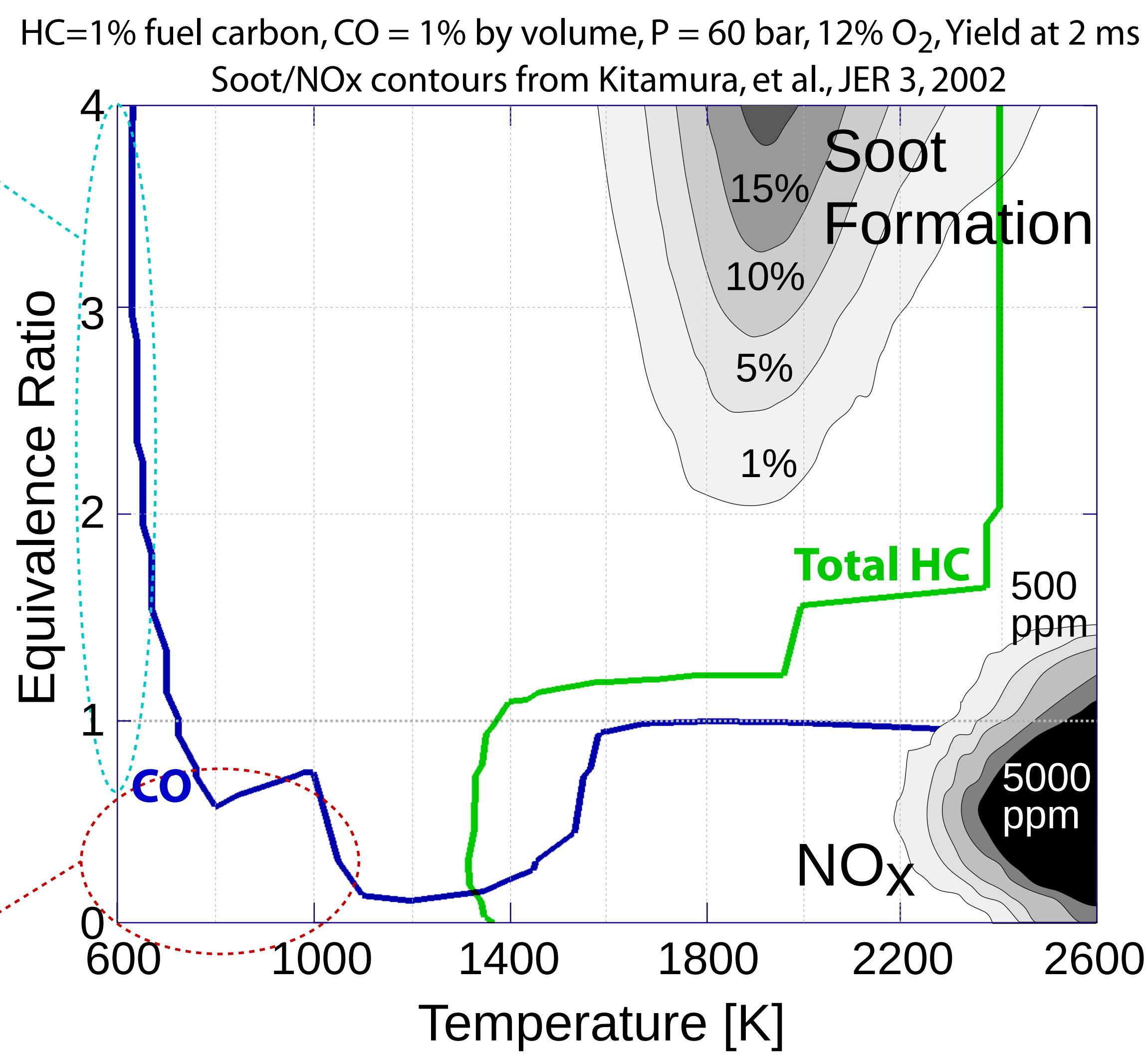
- HCs can be consumed well before CO oxidation is complete

Conversely, high HC but low CO may be observed

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

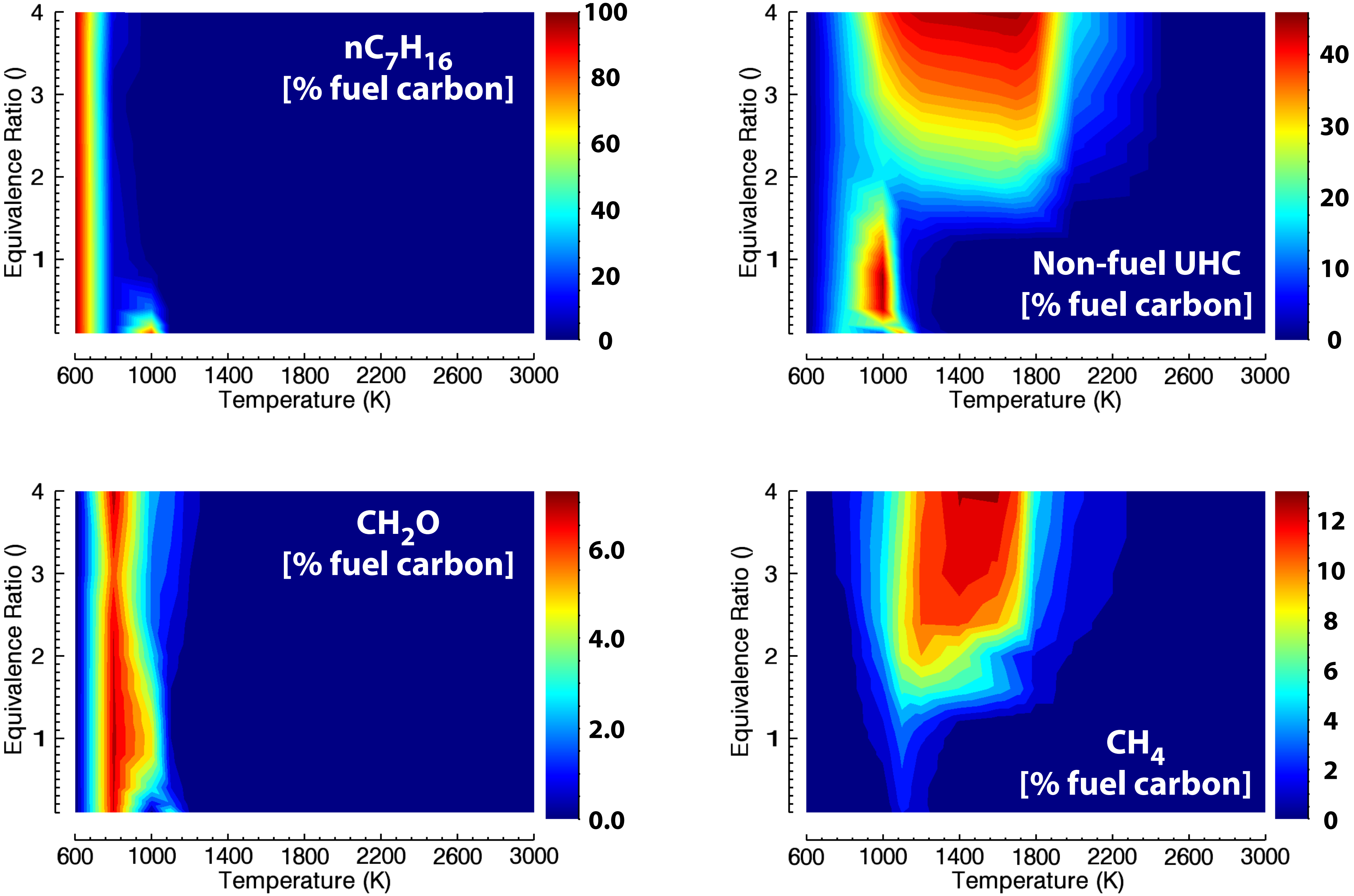
...so can liquid films!





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

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 and engine geometry** (2007-01-0907; Proc. Comb Inst. 31, 2963-2970; 2007-01-1836)

- **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). There is little influence of dilution on UHC emissions in bulk gases.**

- **Boost increases both chemical rates and mixing rates, and can reduce UHC stemming from over-lean as well as over-rich regions (Careful! There may be a soot penalty)** (Colban, et al., SAE 2008)

Closure

- **There is no simple answer to the question "What is the dominant source of CO & UHC emissions 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