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The Co-Optimization of Fuels and Engines: Chemical Kinetics and Optical Research

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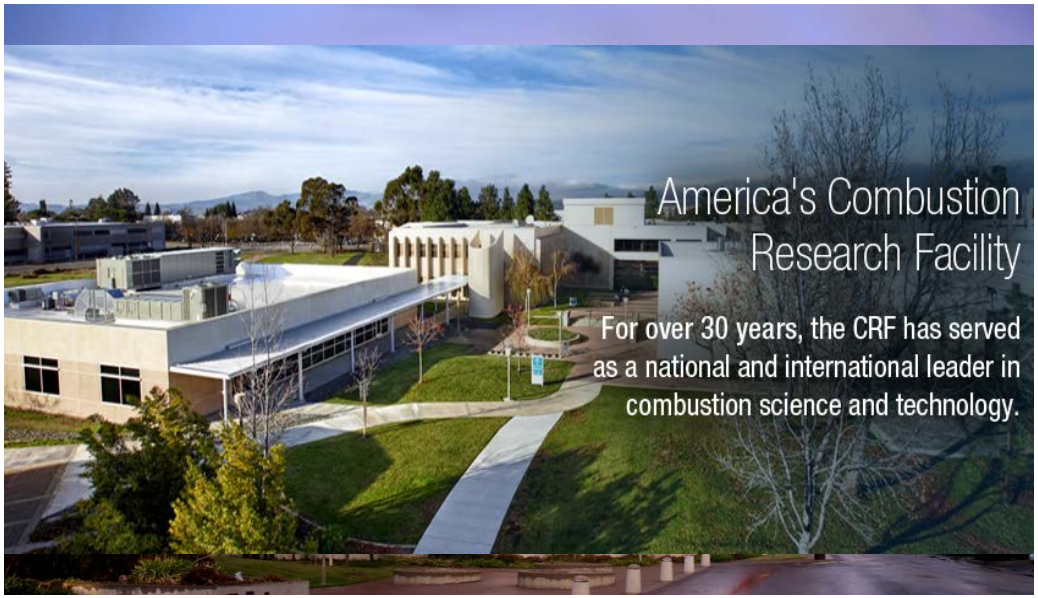
Sponsor: USDOE Office of FreedomCAR and Vehicle Technologies
Program Managers: Gurpreet Singh, Leo Breton, Kevin Stork

Combustion Research Facility
Sandia National Labs, Livermore, California

"The mission of the CRF is to conduct a broad range of basic and applied research and development in combustion science and technology. We aim to improve our nation's ability to utilize and control combustion processes."



- Facility built in 1980
- 100 full-time employees
- 100 visitors per year
  - –**Post-docs**
  - –University faculty
  - –**Undergraduate interns**
  - –**Graduate students**
  - –Industrial collaborators

Visitors bring technical knowledge and skills. The CRF provides access to facility equipment, resources, and a knowledge base of combustion

crf.sandia.gov or Google "Combustion Research Facility"

Part 1: Overview of the US DOE Co-Optimization of Fuels and Engines Project (Co-Optima)

Slide materials from Co-Optima team members

- John Farrell, National Renewable Energy Laboratory, USA
- Dan Gaspar, Pacific Northwest National Laboratory, USA
- Jim Szybist, Oak Ridge National Laboratory, USA
- Paul Miles, Sandia National Laboratories, USA

Co-Optima US Department of Energy management team:

- Kevin Stork, Vehicle Technologies Office
- Gurpreet Singh and Leo Breton, Vehicle Technologies Office
- Alicia Lindauer, Bioenergy Technologies Office

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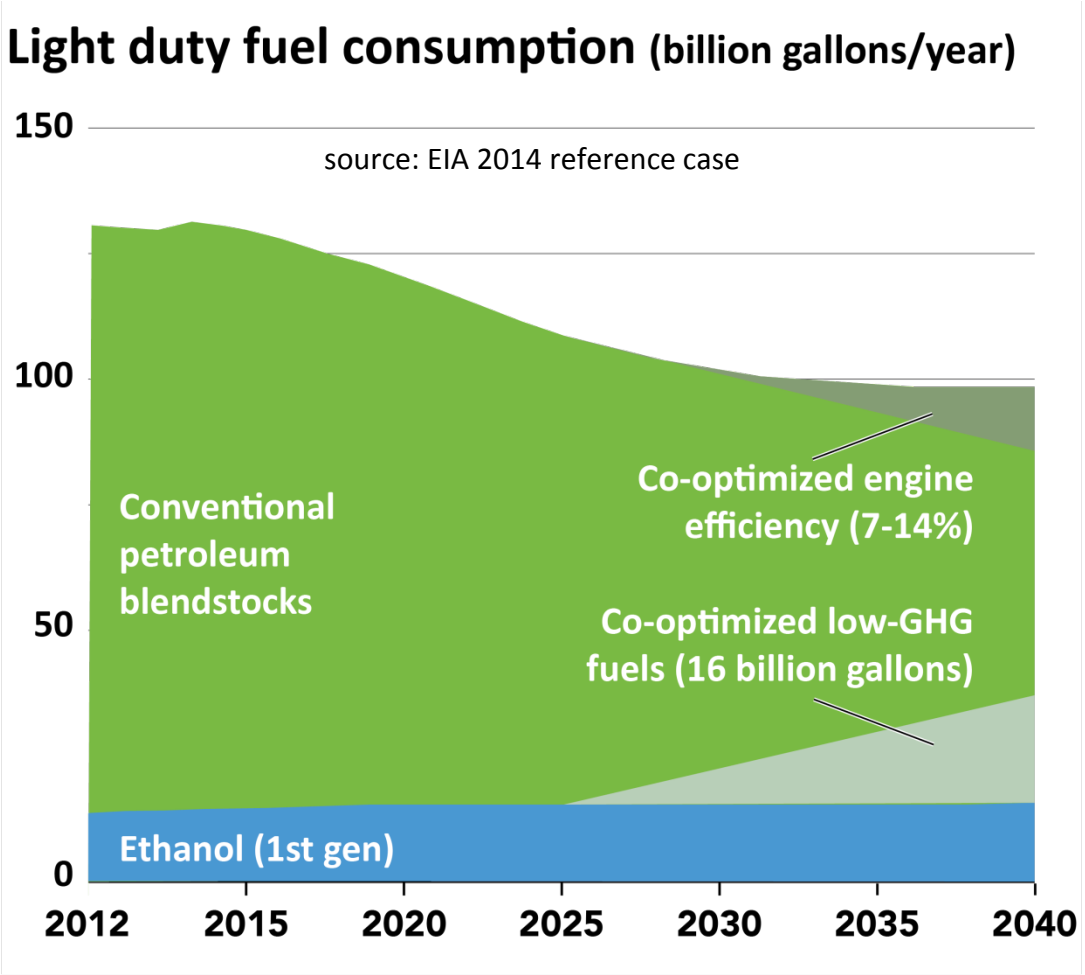
Co-Optimization of Fuels and Engines

- What fuel properties maximize engine performance?
- How do engine parameters affect efficiency?
- What fuel and engine combinations are sustainable, affordable, and scalable?

Better fuels,
Better vehicles,
Sooner

Goal of Co-Optima is to reduce US petroleum usage

Goal: 30% per-vehicle petroleum reduction via efficiency and displacement



Co-Optima targets varied vehicle classes & powertrains

Applicable to **light, medium, and heavy-duty** engines and **hybridized and non-hybridized** powertrains

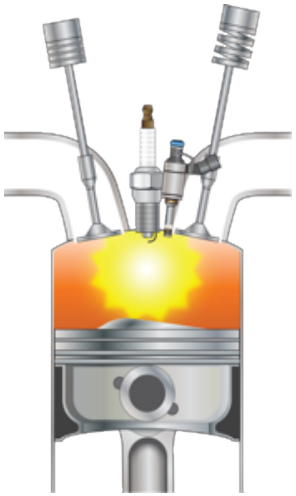
Co-Optima's governing hypotheses for engines & fuels

1. **Central Engine Hypothesis:**
   There are engine architectures and strategies that provide higher thermodynamic efficiencies than available from modern internal combustion engines; new fuels are required to maximize efficiency and operability across a wide speed/load range.

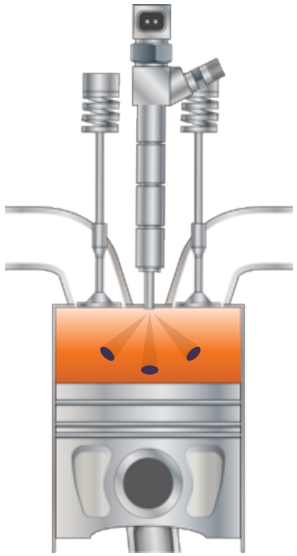
2. **Central Fuel Hypothesis:**
   If we identify target values for the critical fuel properties that maximize efficiency and emissions performance for a given engine architecture, then fuels that have properties with those values (regardless of chemical composition) will provide comparable performance.

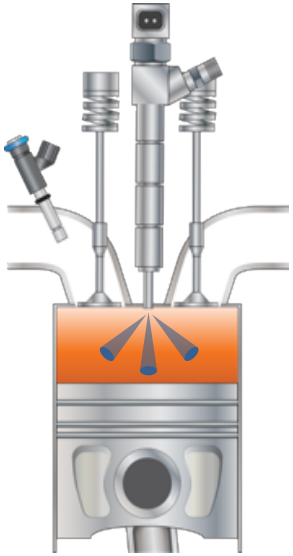
Co-Optima has two parallel efforts in SI and ACI engines

Thrust I: Spark Ignition (SI)	Thrust II: Advanced Compression Ignition (ACI) kinetically-controlled and compression-ignition combustion

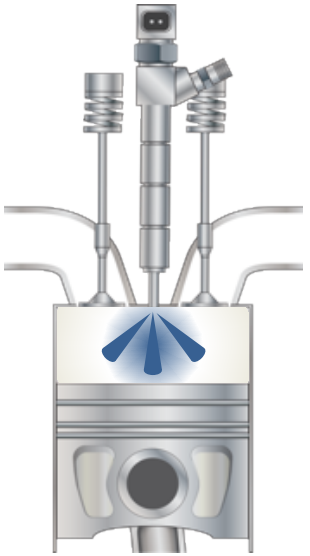


Low reactivity fuel



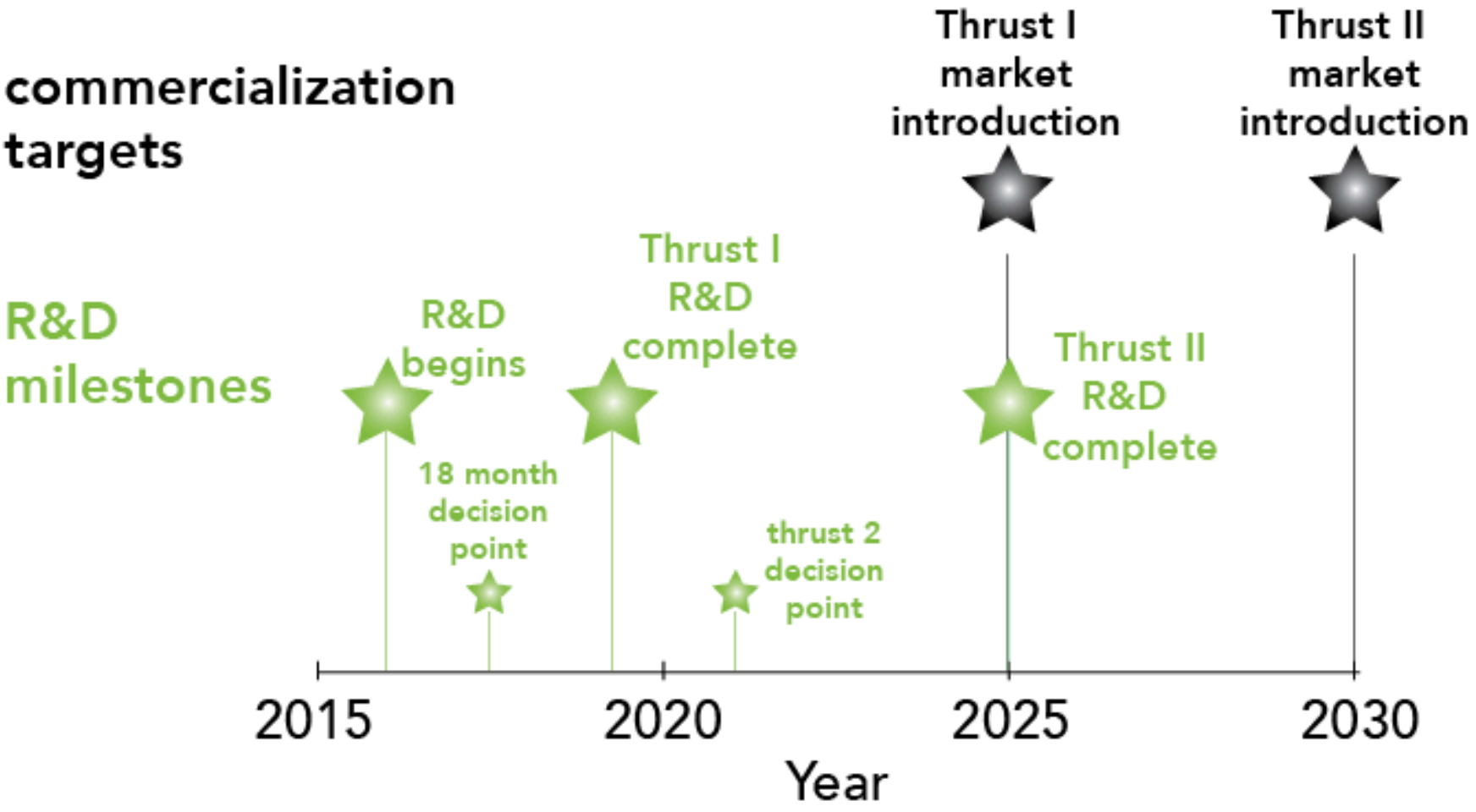


Range of fuel properties TBD



High reactivity fuel

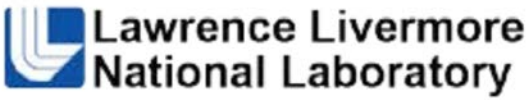
Co-Optima R&D timeline and commercialization targets



US DOE Co-Optima project involves 9 US national labs

US Department of Energy (DOE)

- Office of Vehicle Technologies
- Office of Bioenergy Technologies



Six Co-Optima teams in end-to-end R&D approach

Low Greenhouse Gas Fuels

Identify promising bio-derived blendstocks, develop selection criteria for fuel molecules, and identify viable production pathways

Fuel Properties

Identify critical properties and allowable ranges, systematically catalogue properties, and predict fuel blending behavior

Advanced Engine Development

Quantify interactions between fuel properties and engine design and operating strategies – enable optimal design of efficient, emission-compliant engines

Modeling and Simulation Toolkit

Extend the range, confidence and applicability of engine experiments by leveraging high-fidelity simulation capabilities

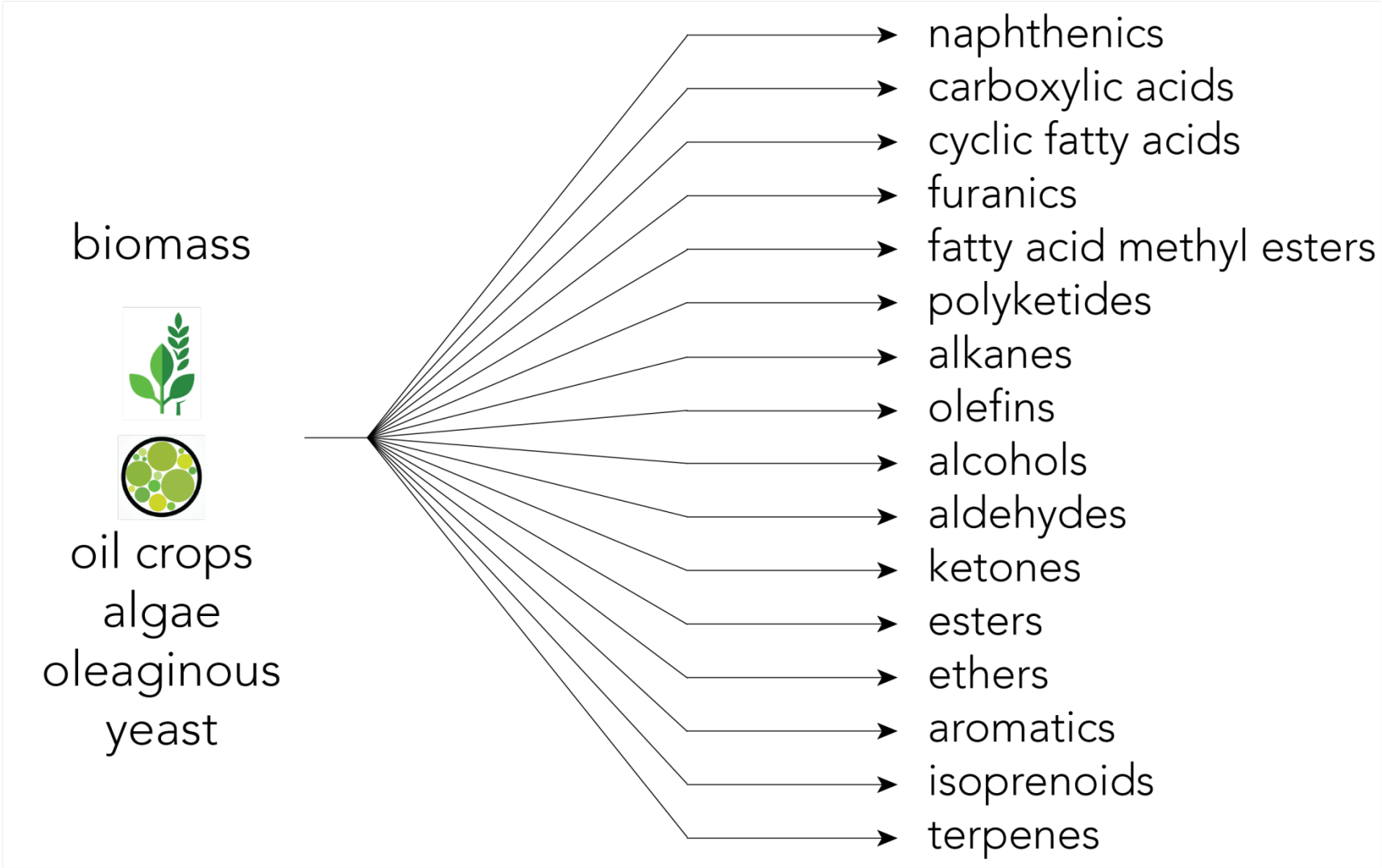
Analysis of Sustainability, Scale, Economics, Risk, and Trade

Analyze energy, economic, and environmental benefits at US economy-level and examine routes to feedstock production at scale through existing biomass markets

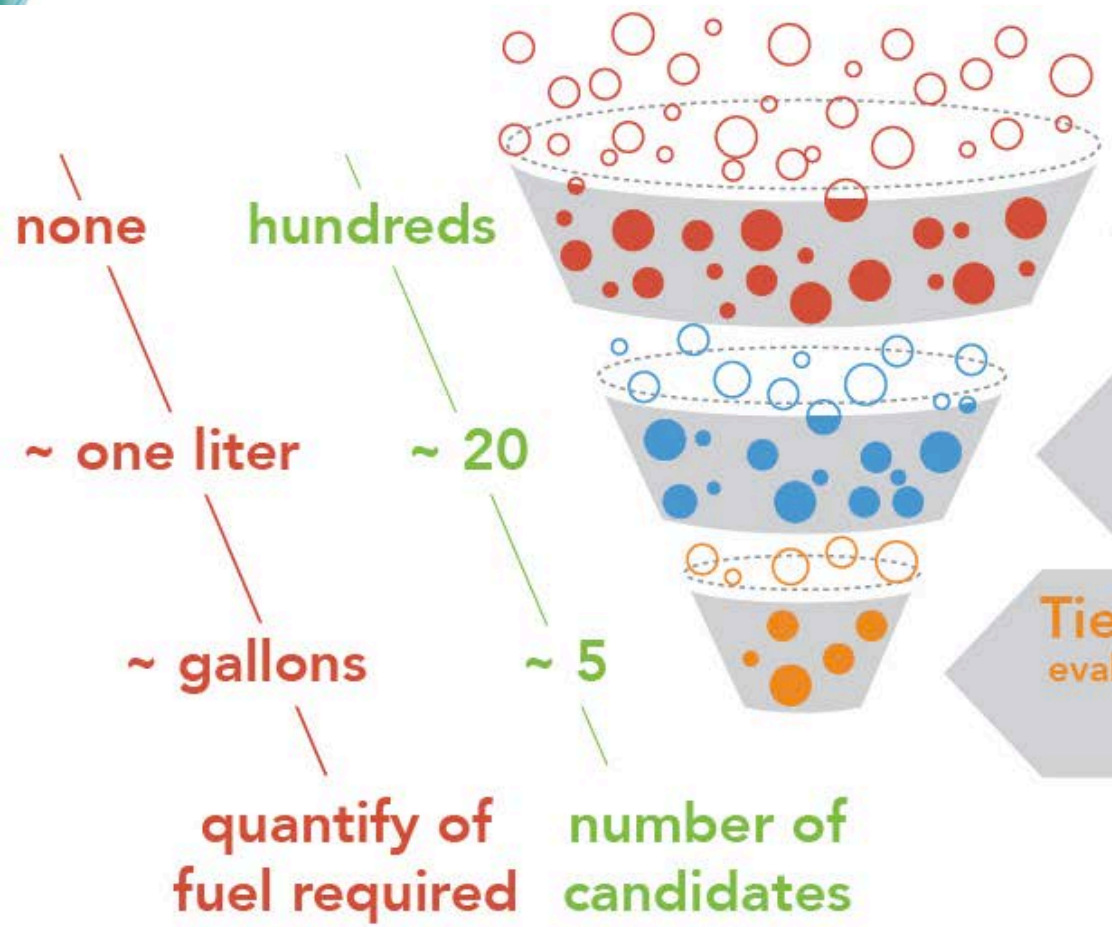
Market Transformation

Identify and mitigate challenges of moving new fuels and engines to markets and engage with full range of stakeholders

A wide range of bio-blendstock classes can be made



Down-selection of bio-blendstocks progresses in 3 tiers



Tier 1: high-level screening

boiling point	corrosivity
freezing point	toxicity
solubility	heteroatom conc.
ignition quality	etc.

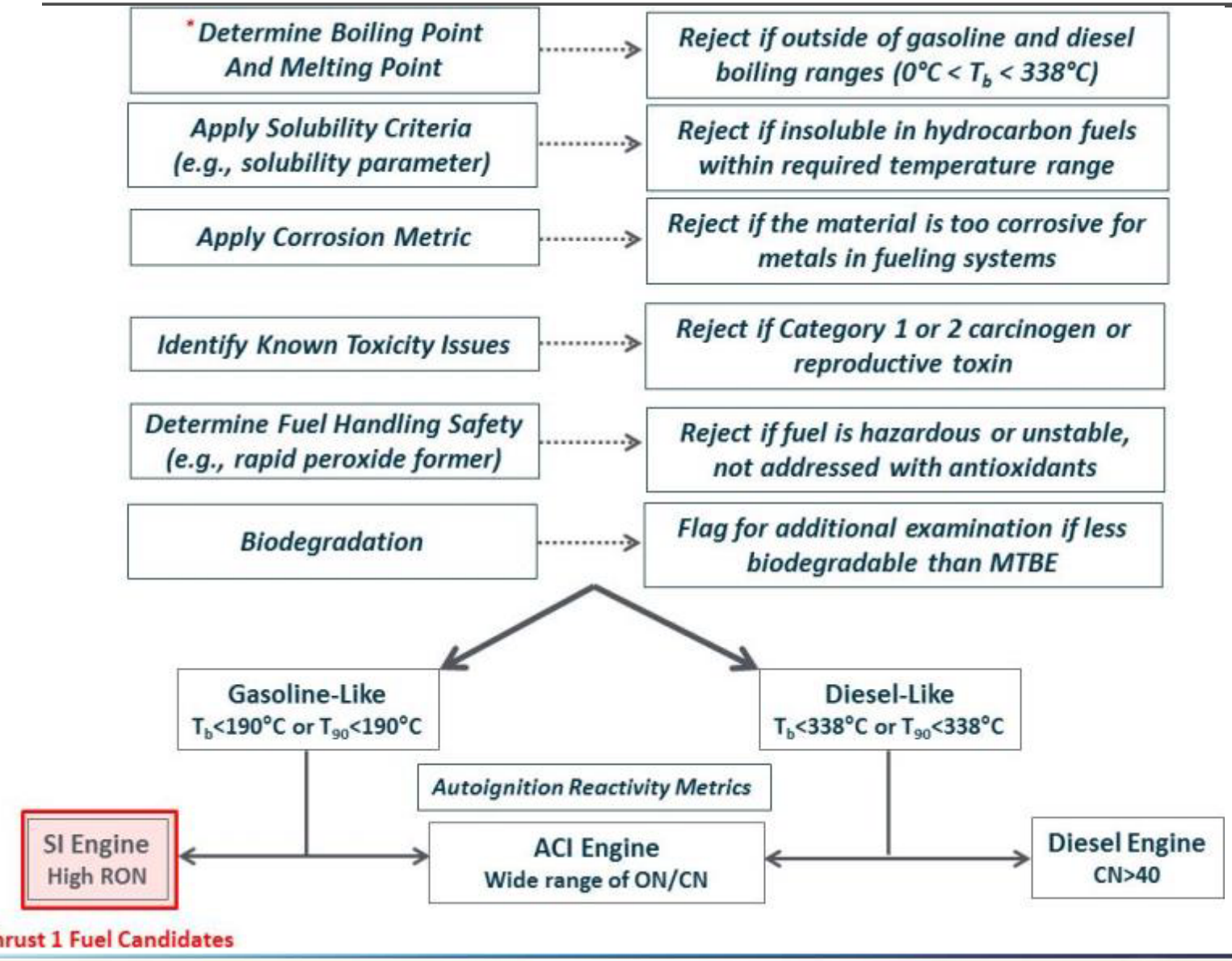
Tier 2: candidate selection

fuel merit function *	state of technology
life cycle GHG	infrastructure compatibility
land use, water	flash point, flammability
economics	etc.

Tier 3: candidate evaluation

evaluate promising candidates in engine tests

Tier 1 screening applies high-level criteria



20 bio-blendstocks of the Tier 2 candidate selection

Alcohols	
0	Ethanol (Reference)
1	Methanol
2	1-butanol
3	2-methyl-butanol
4	2-butanol
5	Isobutanol (2-methylpropan-1-ol)
6	Guerbet alcohol mixture
Alkanes	
7	2,2,3-trimethyl-butane
Esters	
8	Acetic acid, methyl ester (methyl acetate)
9	Acetic acid, ethyl ester (ethyl acetate)
10	Acetic acid, butyl ester (butyl acetate)
11	Anaerobic acid fermentation and esterification mixture

Furans	
12	2,5-dimethylfuran / 2-methylfuran mixture
Ketones	
13	2-pentanone
14	Methylethylketone (2-butanone)
Alkenes	
15	Isooctene
Aromatics	
16	Vertifuel (60%+ aromatics)
17	Fractional condensation of sugars + upgrading
18	Methanol-to-gasoline
19	Catalytic fast pyrolysis
20	Catalytic conversion of sugars

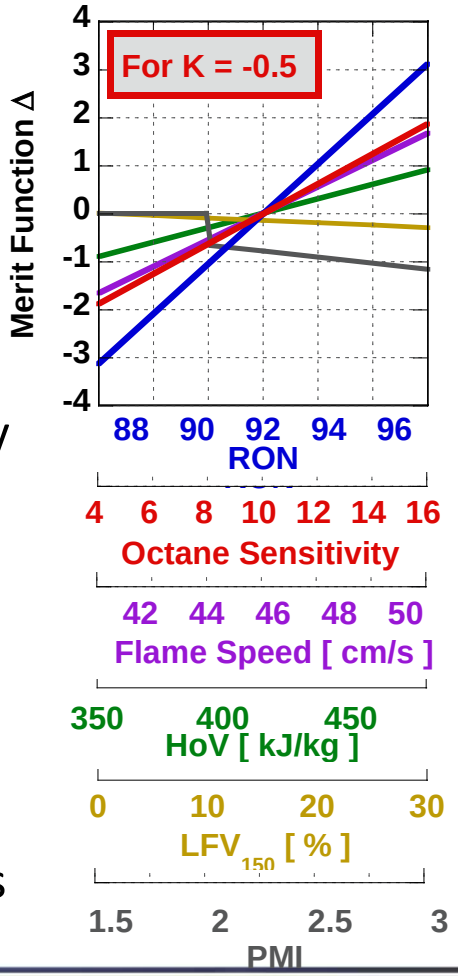
Efficiency merit function is a rough fuel-ranking tool

$$Merit = \sum \frac{(RON_{mix} - 92)}{1.6} - K\frac{(S_{mix} - 10)}{1.6} + \frac{(S_{L\,mix} - 46[cm/s])}{3} + \frac{0.01[ON/kJ/kg](HoV_{mix} - 415)[kJ/kg]}{1.6} + \frac{(HoV_{mix} - 415)[kJ/kg]}{130} - LFV_{150} - H(PMI - 2.0)[0.67 + 0.5(PMI - 2.0)]$$

RON | Octane Sensitivity | Flame Speed | Heat of Vaporization (HoV) | Distillation | Particulate Emissions

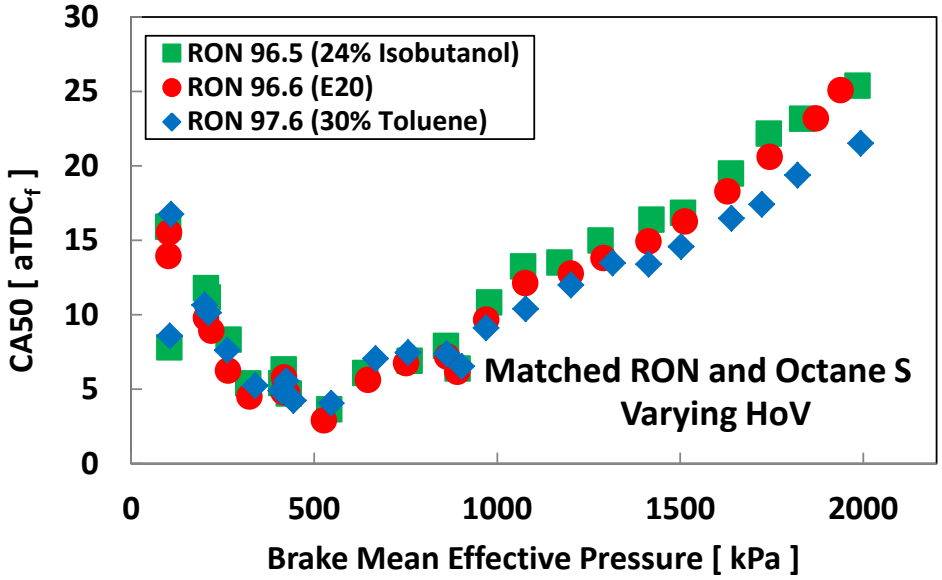
Thrust I Engine Research: *Develop a robust and quantitative understanding of how fuel properties affect efficiency*

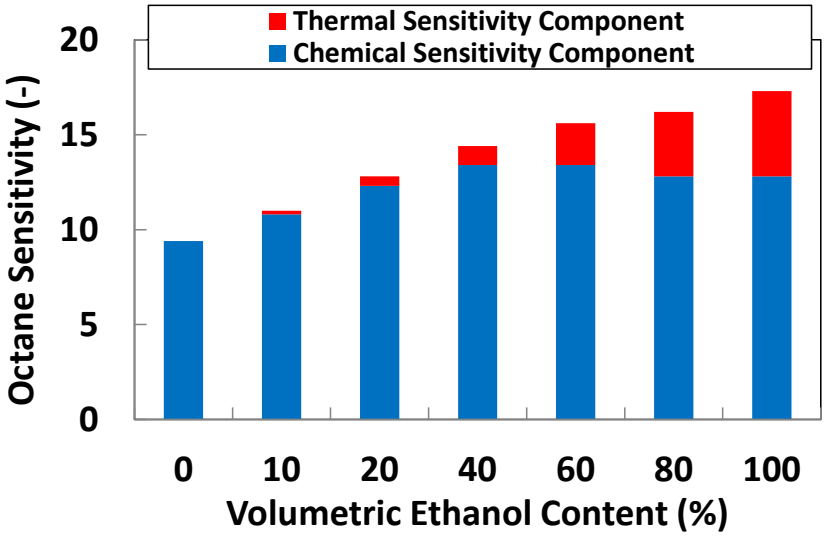
- Merit function: quantify how fuel properties affect efficiency
- Merit function is not finalized – still developing
  - Are these the right fuel properties?
  - Are their effects properly quantified?
- We'll test the central fuel hypothesis using biofuels with different structures / functional groups than petroleum fuels



New Co-Optima data help settle Thrust I (SI) role of HoV

- Previous studies co-varied heat of vaporization (HoV) and octane sensitivity (S); results are inconsistent about HoV impact on knock
  - Negligible impact on knock-limited spark advance and efficiency (SAE 2014-01-1228)
  - HoV linearly increases effective octane rating (SAE 2012-01-1284)
  - HoV effects already included in RON test (SAE 2012-01-1277, SAE 2013-01-0886)
- New Co-Optima HoV experiments hold RON & S constant (SAE 2016-01-0836)
  - Main conclusion: RON & S dominate over HoV over ranges typical of most fuels
  - Ethanol HoV effects on knock are negligible relative to RON & S below E20

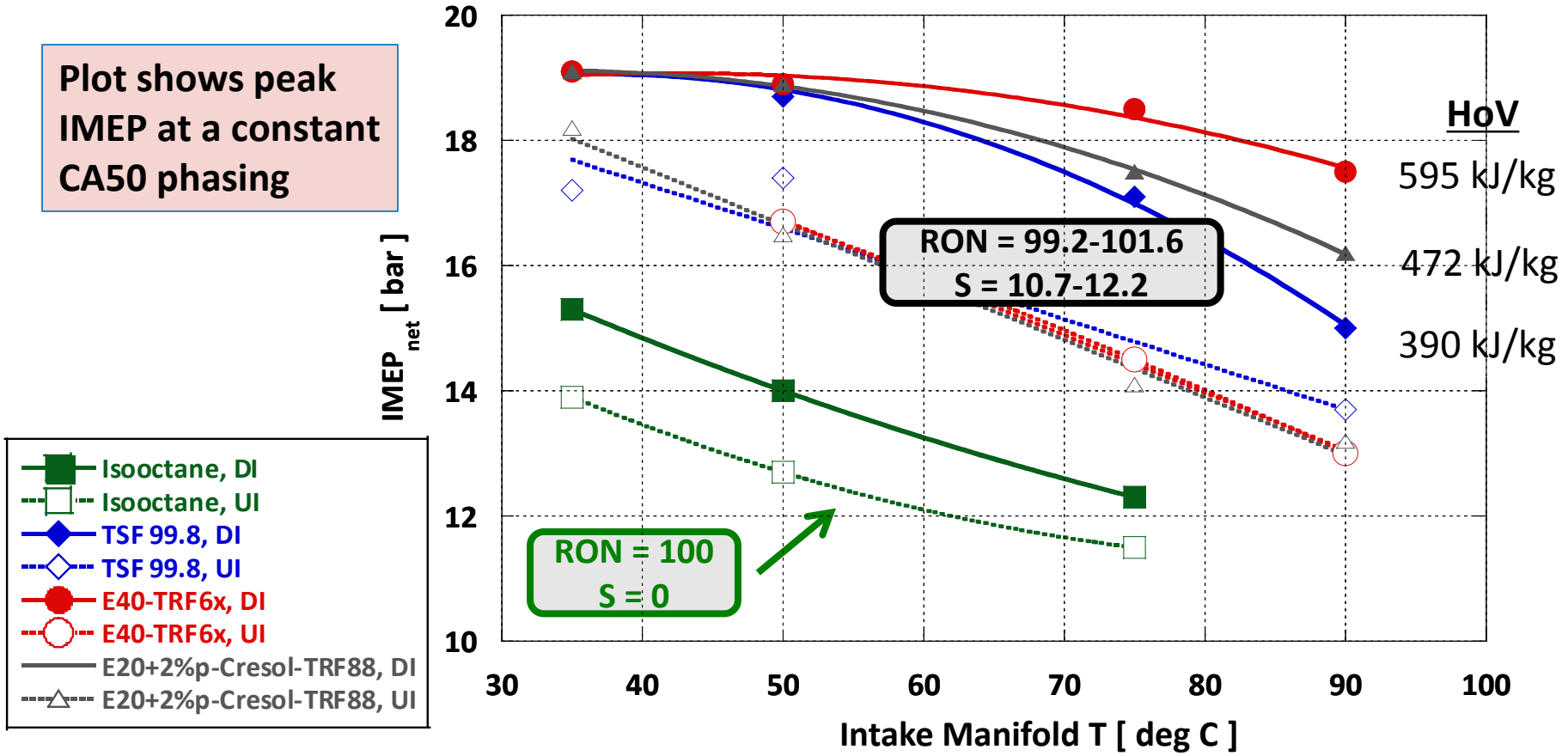




HoV can be important for DI at high intake temperatures

- Upstream injected (UI) 100 RON, S ≈ 11 fuels have higher peak IMEP at constant CA50 than iso-octane (RON 100, S =0), and HoV has little effect (S is dominant)
- Direct injection (DI) of iso-octane has HoV benefit, but less than S ≈ 11 effect
- DI of S ≈ 11 fuels also has HoV benefit, which increases with manifold temp.

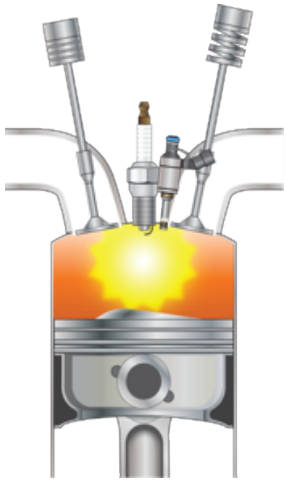
Plot shows peak IMEP at a constant CA50 phasing



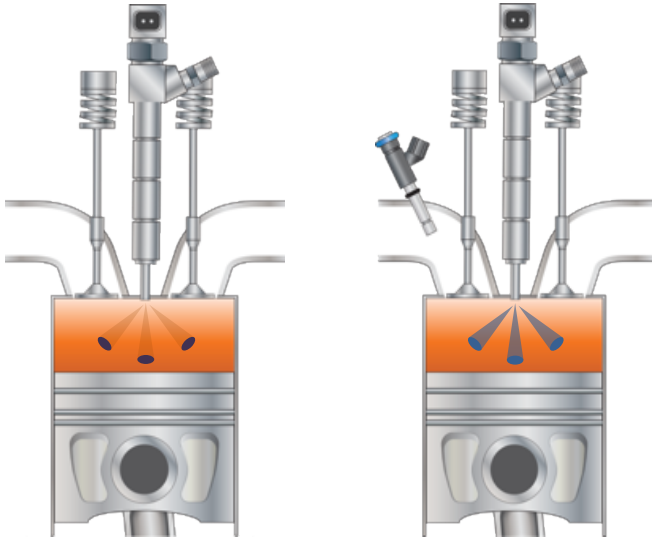
Part 2: Chemical kinetics and optical diagnostics research for advanced compression ignition engines

- Co-Optima's Thrust II encompasses both gasoline-like and diesel-like fuels
- Examines possibility of using Thrust I fuels in Thrust II engines
- Use new fuels to accelerate Thrust II technology development
- **Chemical-kinetic processes of ignition and combustion are critical**

Thrust I: Spark Ignition (SI)	Thrust II: Advanced Compression Ignition (ACI) kinetically-controlled and compression-ignition combustion



Low reactivity fuel



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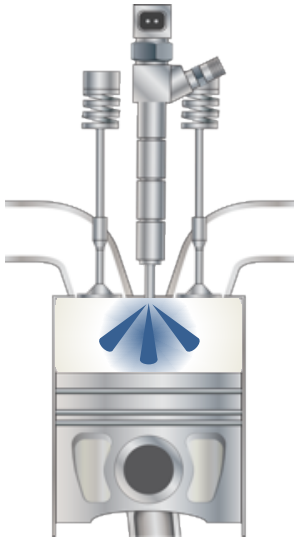
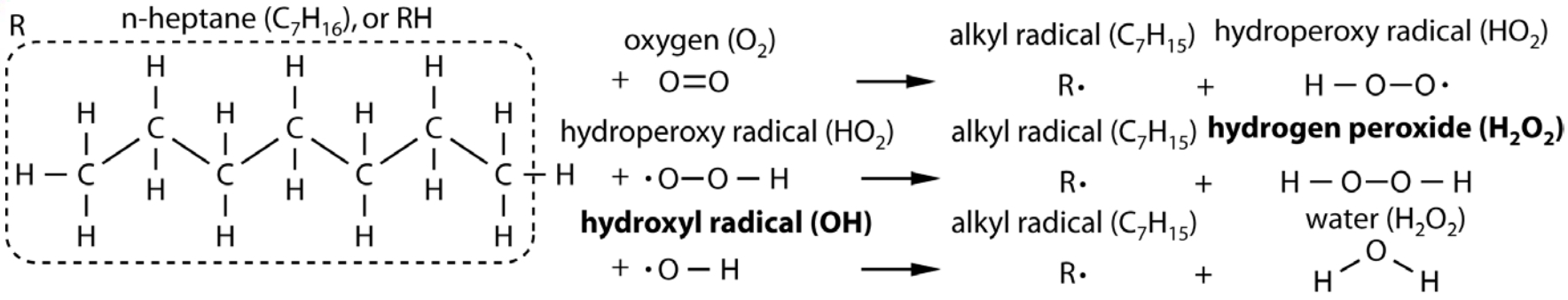


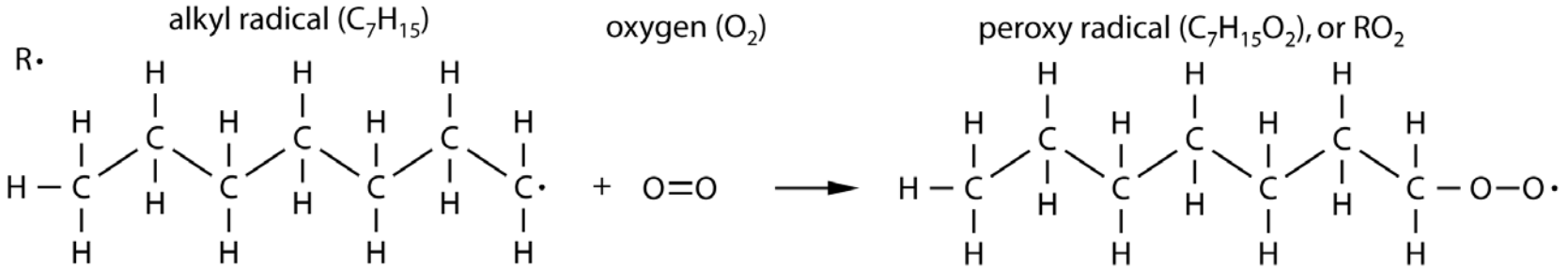
High reactivity fuel

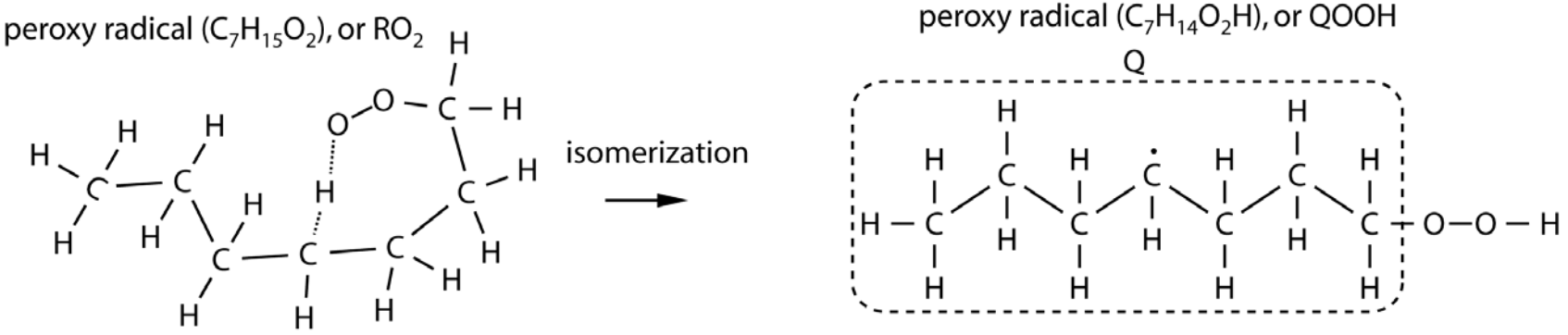
n-heptane chemical kinetics as an example of autoignition and combustion in LTC/ACI engines

- n-heptane (C_7H_{16}) is a paraffinic fuel component with low-temperature chemistry typical of high-cetane (low octane) hydrocarbon fuels
- Closed-reactor 0-dimensional simulations using n-heptane as a surrogate for diesel-like fuels has yielded valuable insight into low-temperature combustion (LTC) autoignition and pollutant formation processes in advanced compression ignition (ACI) engines
- The following seven slides are based on work at Lawrence Livermore National Laboratory (Curran, H. J., P. Gaffuri, W. J. Pitz, and C. K. Westbrook, "A Comprehensive Modeling Study of n-Heptane Oxidation" Combustion and Flame 114:149-177, 1998)

First step is low-temperature pre-ignition (T<900 K): One OH consumed + isomerization

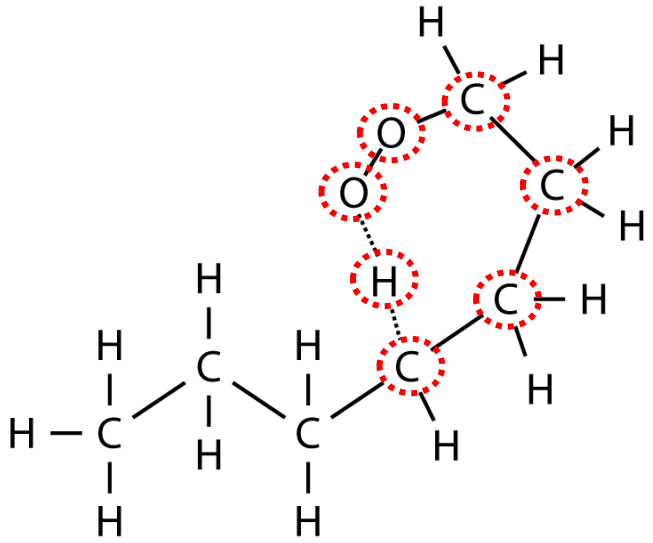




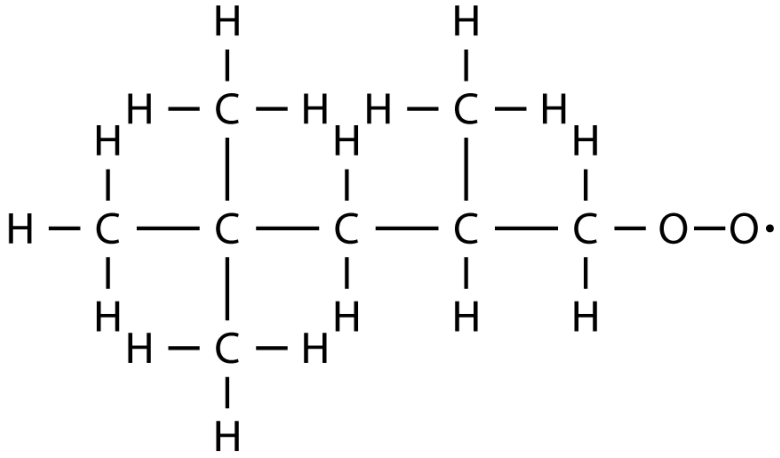


Straight-chain hydrocarbons (diesel) isomerize more quickly than branched hydrocarbons (gasoline)

n-heptane peroxy radical ($C_7H_{15}O_2$), or RO_2

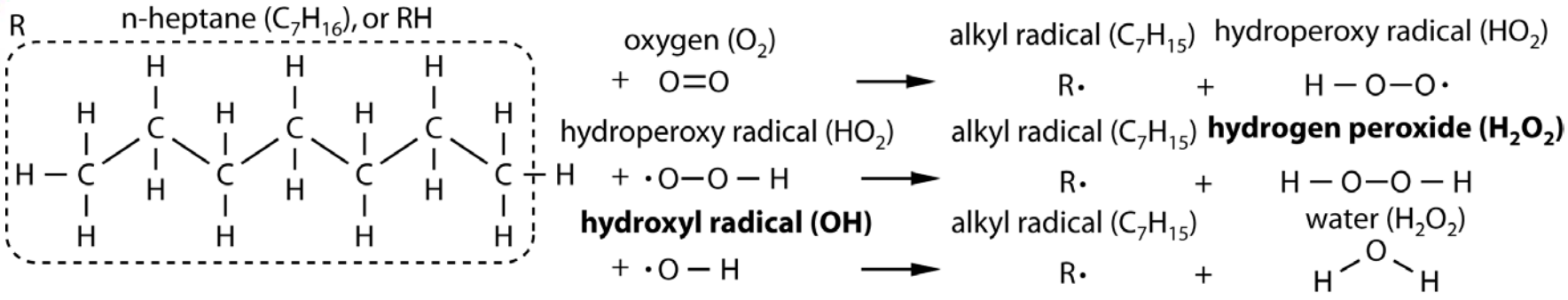


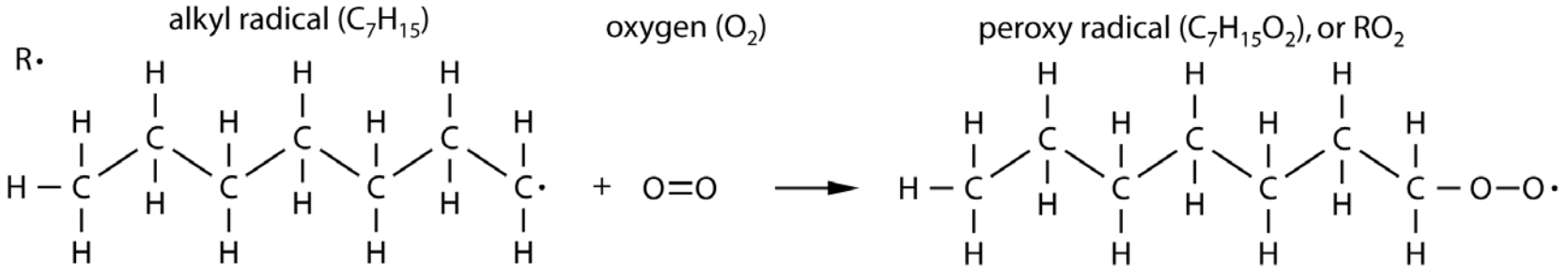
iso-octane peroxy radical ($C_8H_{17}O_2$)

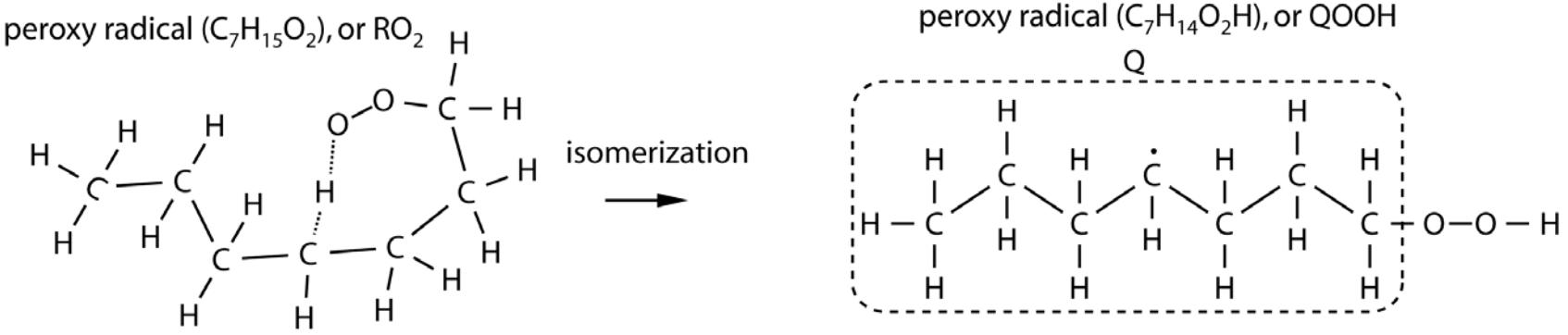


"7-member ring"

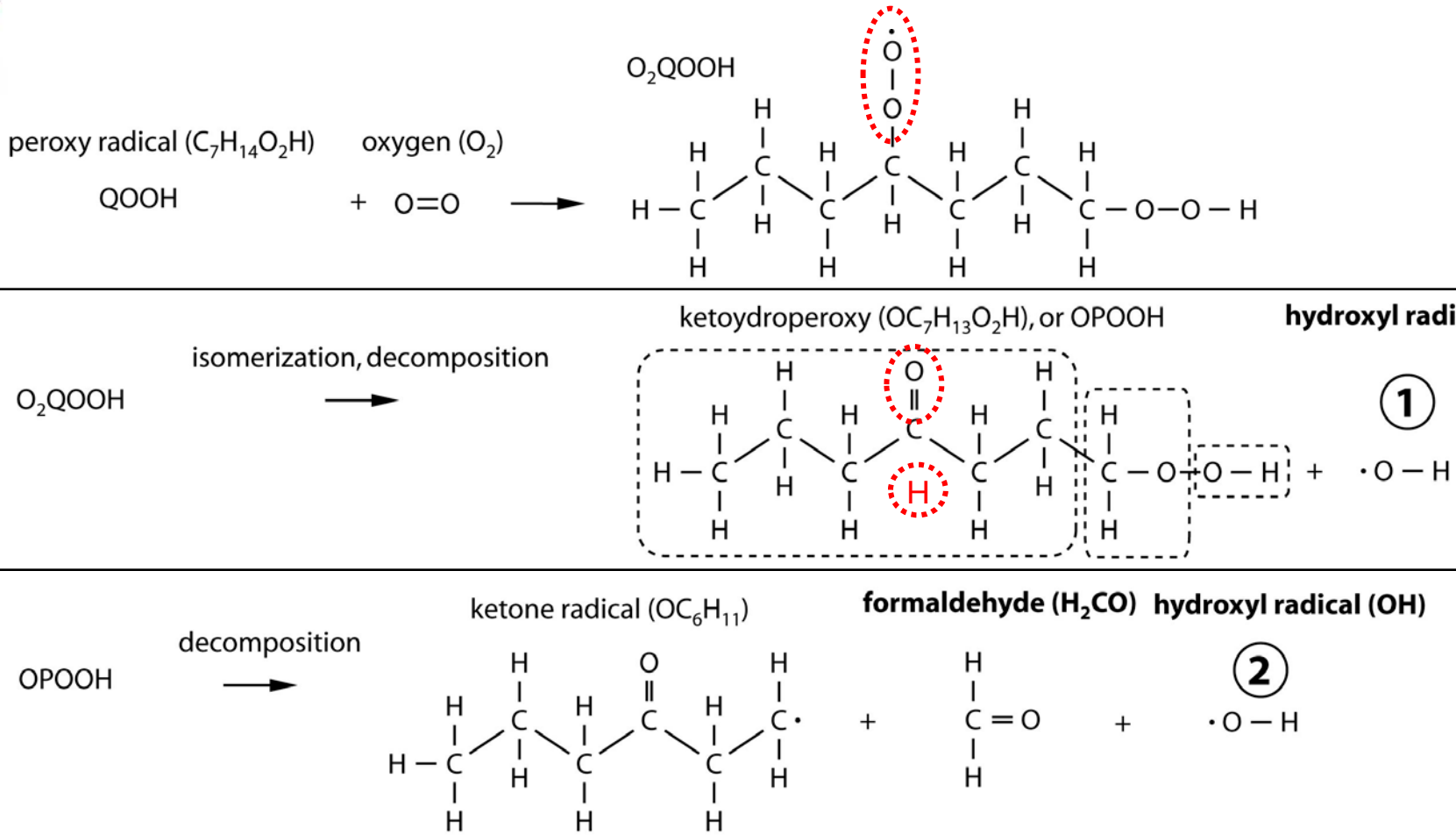
First step is low-temperature pre-ignition (T<900 K): One OH consumed + isomerization



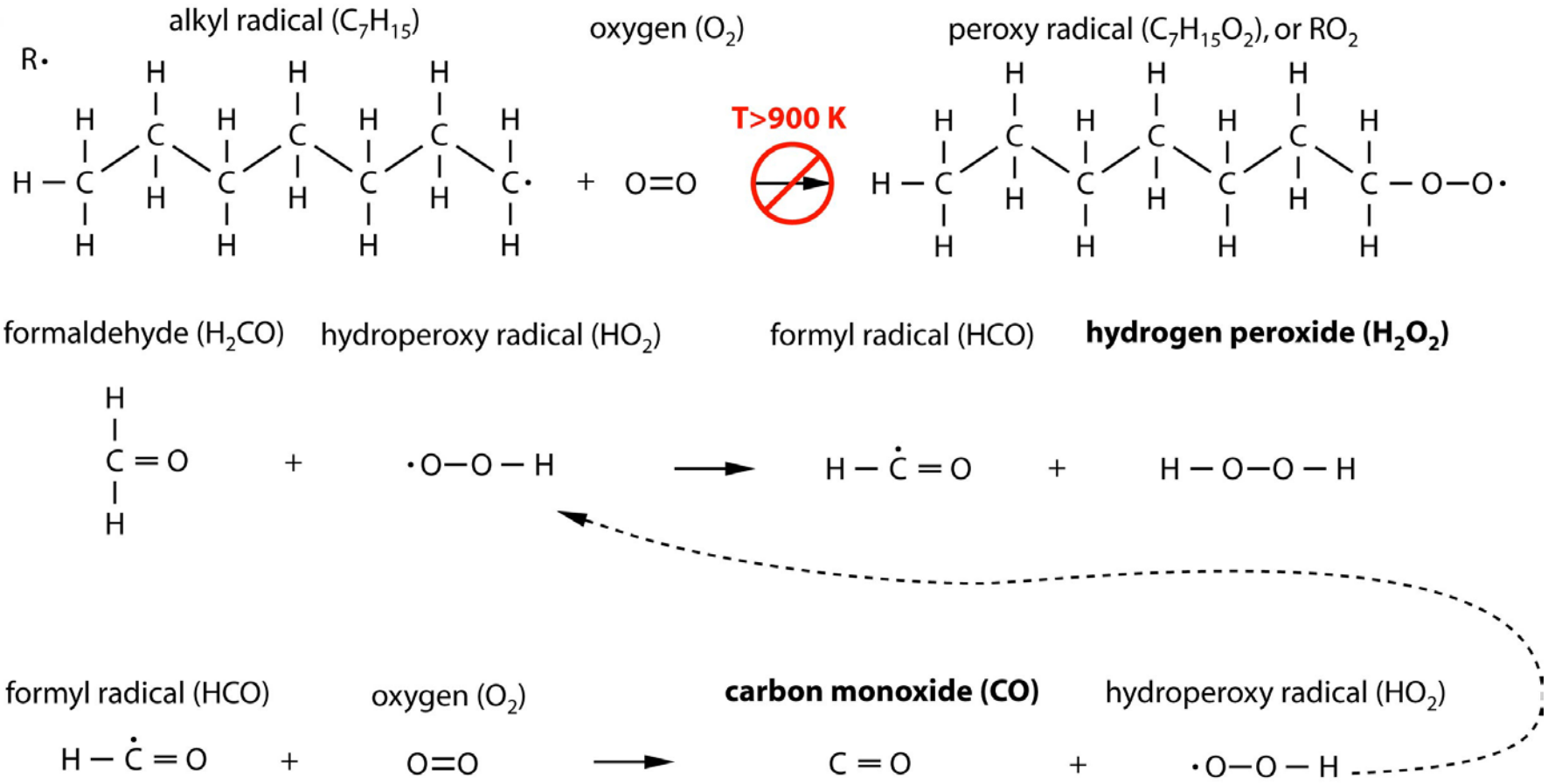




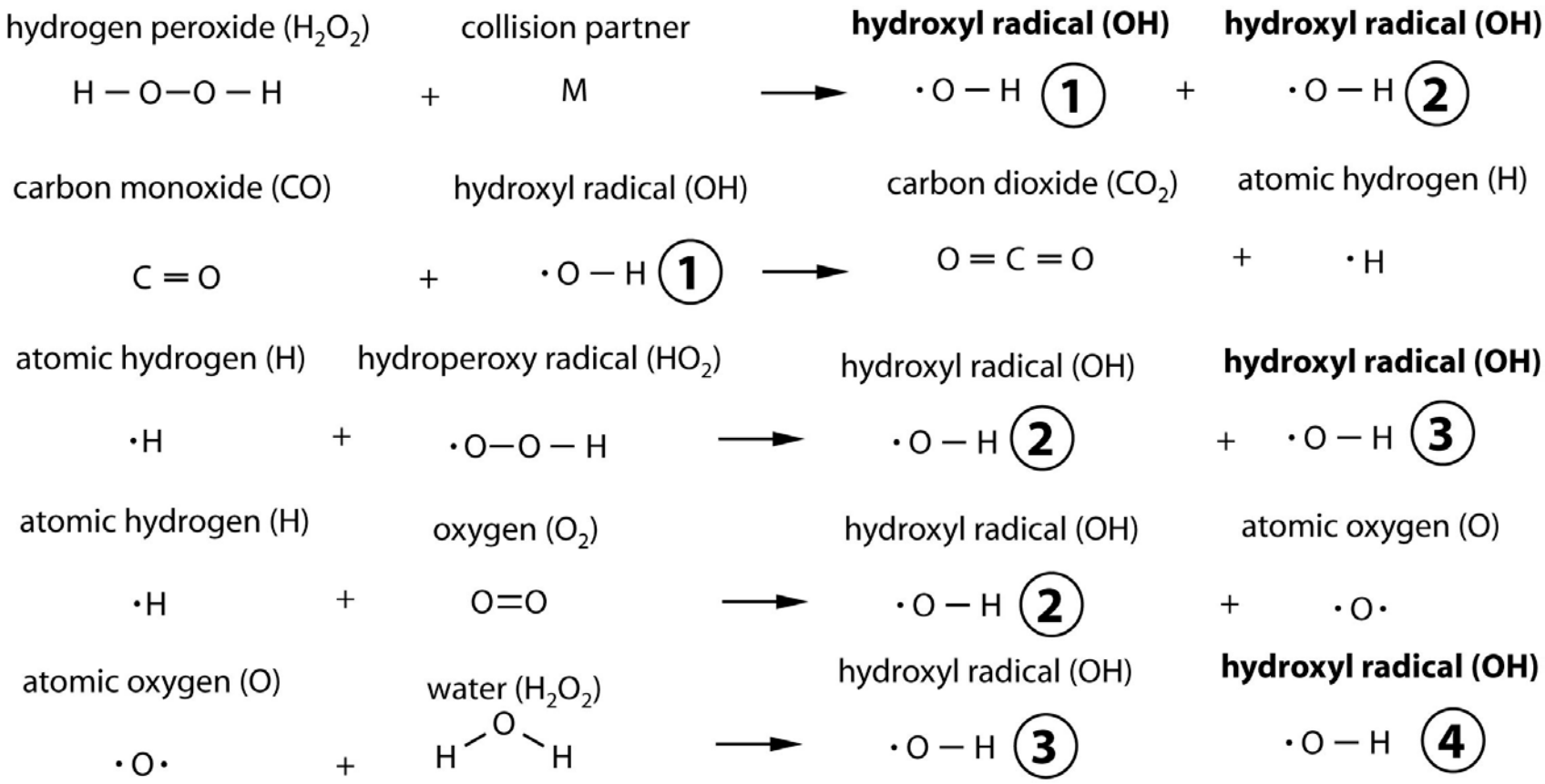
Second step is first-stage ignition (T<900 K): Two OH produced + formaldehyde



Third step is intermediate temperature pre-ignition (900<T<1200 K): Consume H_2CO, build CO & H_2O_2

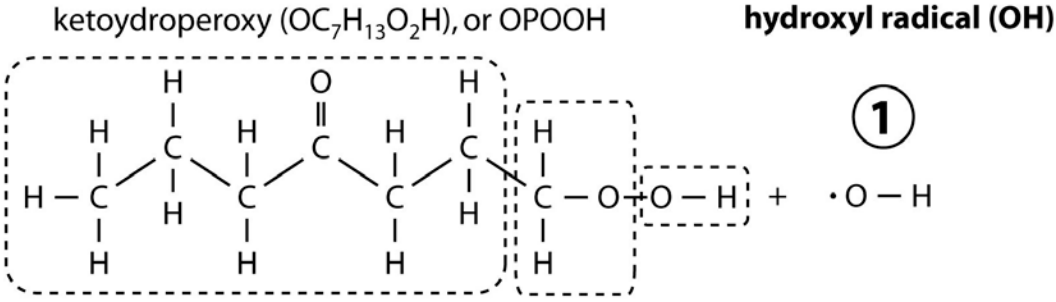


Fourth step is second-stage ignition (T>1200 K): H_2O_2 decomposition leads to OH runaway



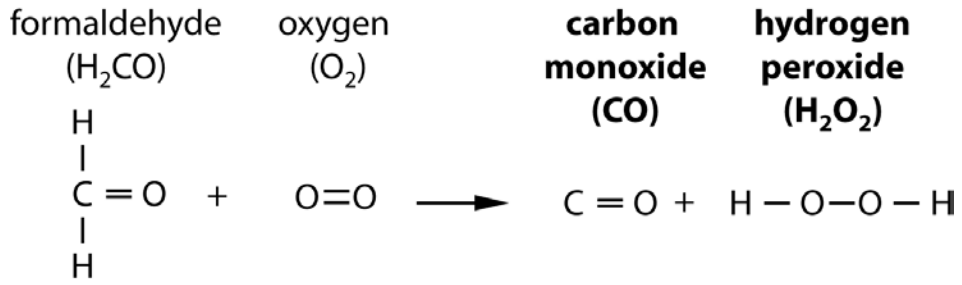
Summary: n-heptane ignition in four steps

1. T<900 K: O_2 and OH attack fuel to make two OH for each OH consumed, so reaction rate increases

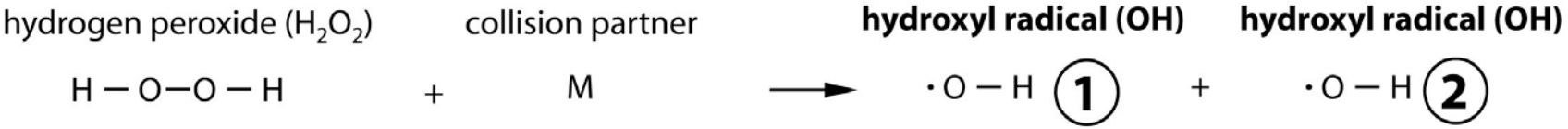


2. First-stage ignition: Reaction runs away as OH concentrations and T rise. Fuel decomposition builds a **pool of formaldehyde** (H_2CO).

3. 900K<T<1200 K: O_2+fuel-radical step shuts down, & low-T reaction chain ends. **Formaldehyde pool** is converted to build pools of CO and hydrogen peroxide (H_2O_2), gradually raising T.



4. Second-stage ignition: Hydrogen peroxide (H_2O_2) decomposes into OH fragments and CO oxidation yields **more OH** as T increases rapidly.

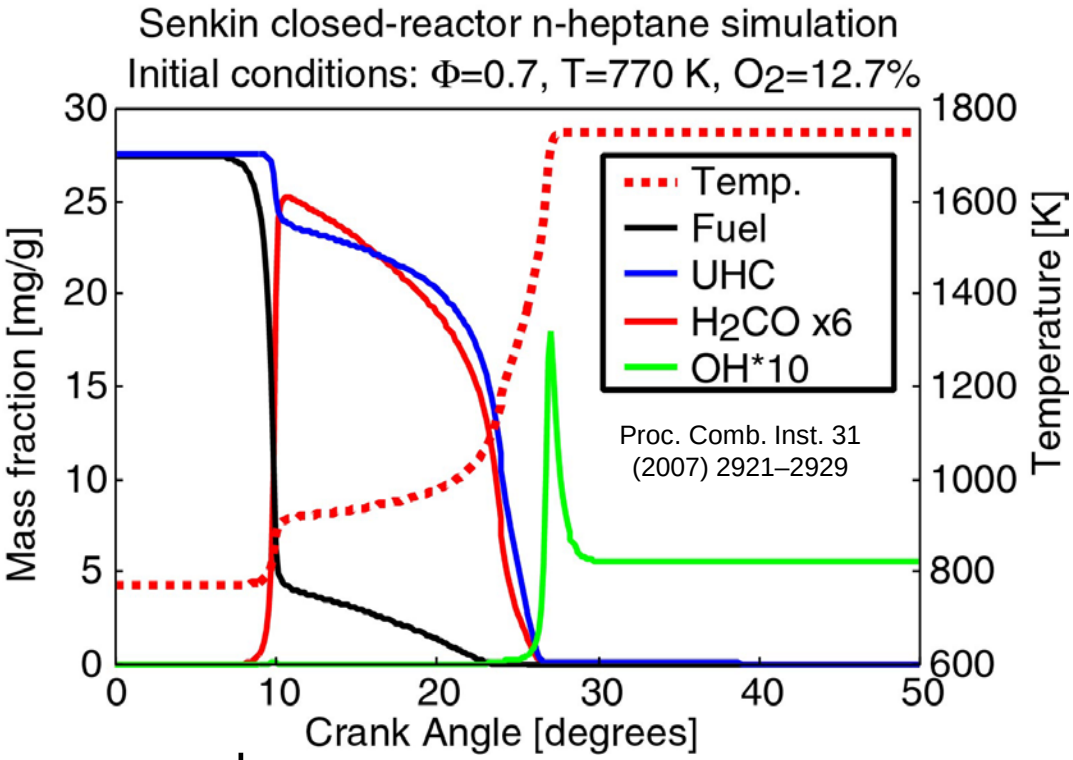


Formaldehyde is a naturally occurring tracer for fuel between first and second stages of ignition

Closed-reactor CHEMKIN simulation of n-heptane ignition using the Lawrence Livermore National Laboratories detailed mechanism of Curran, Pitz, and Westbrook

First-Stage (10 CAD):

- Much of the **parent fuel molecule (black)** reacts, and a "soup" of **UHCs (blue)** is formed
- **Formaldehyde (H_2CO, red) can track the soup of UHC (blue)**



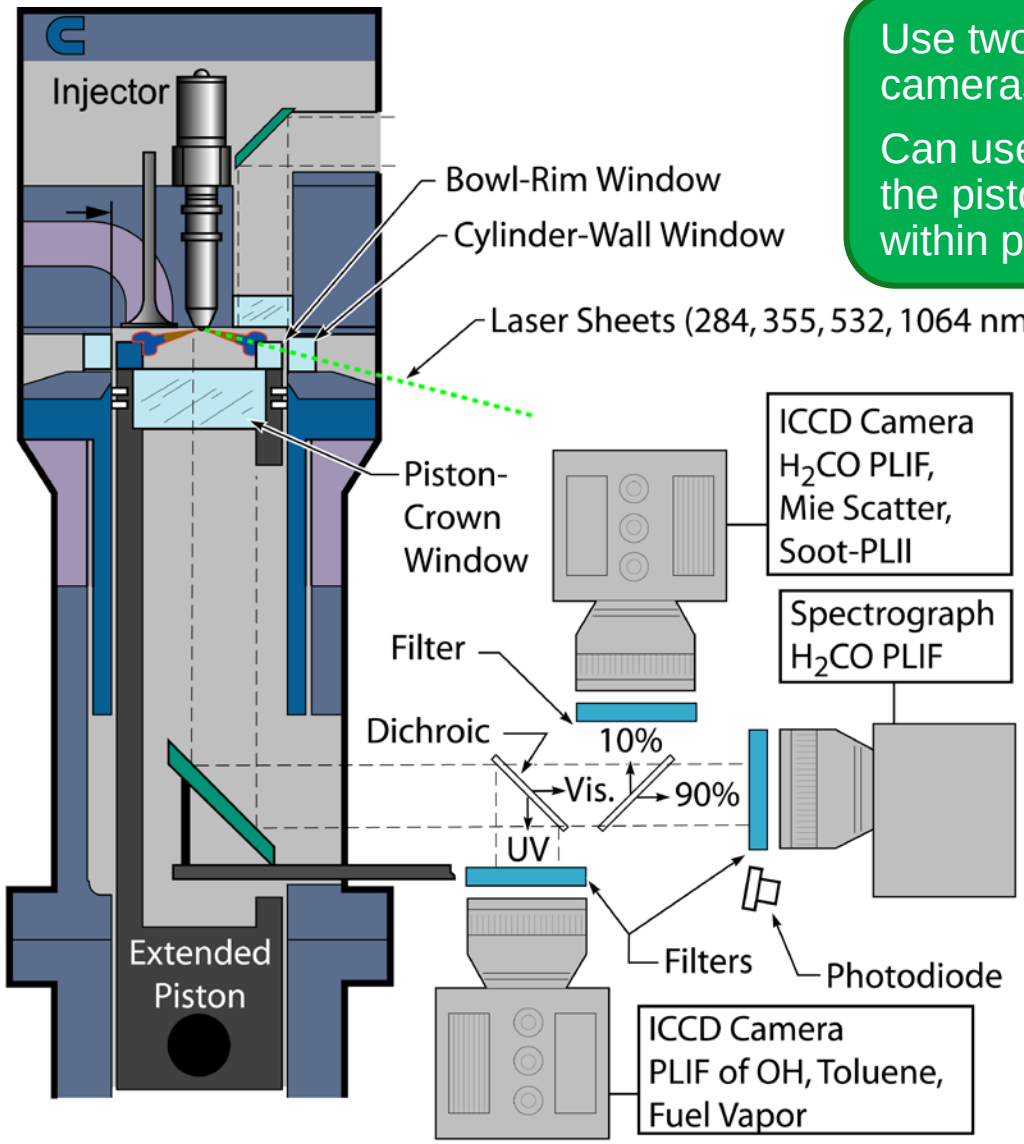
Second-Stage (25 CAD):

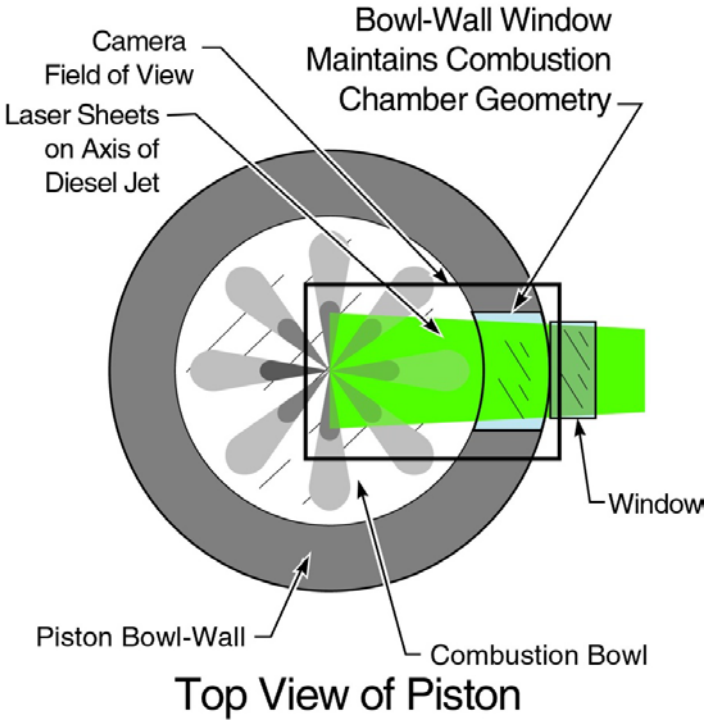
- Nearly all **UHC** and **H_2CO** consumed
- **Appearance of OH (green) marks hot ignition and consumption of UHC**

Simultaneous laser/imaging diagnostics

Use two overlapped laser-sheets and two cameras for simultaneous imaging

Can use either a cut-out or a window in the piston bowl-wall to allow laser access within piston bowl of combustion chamber





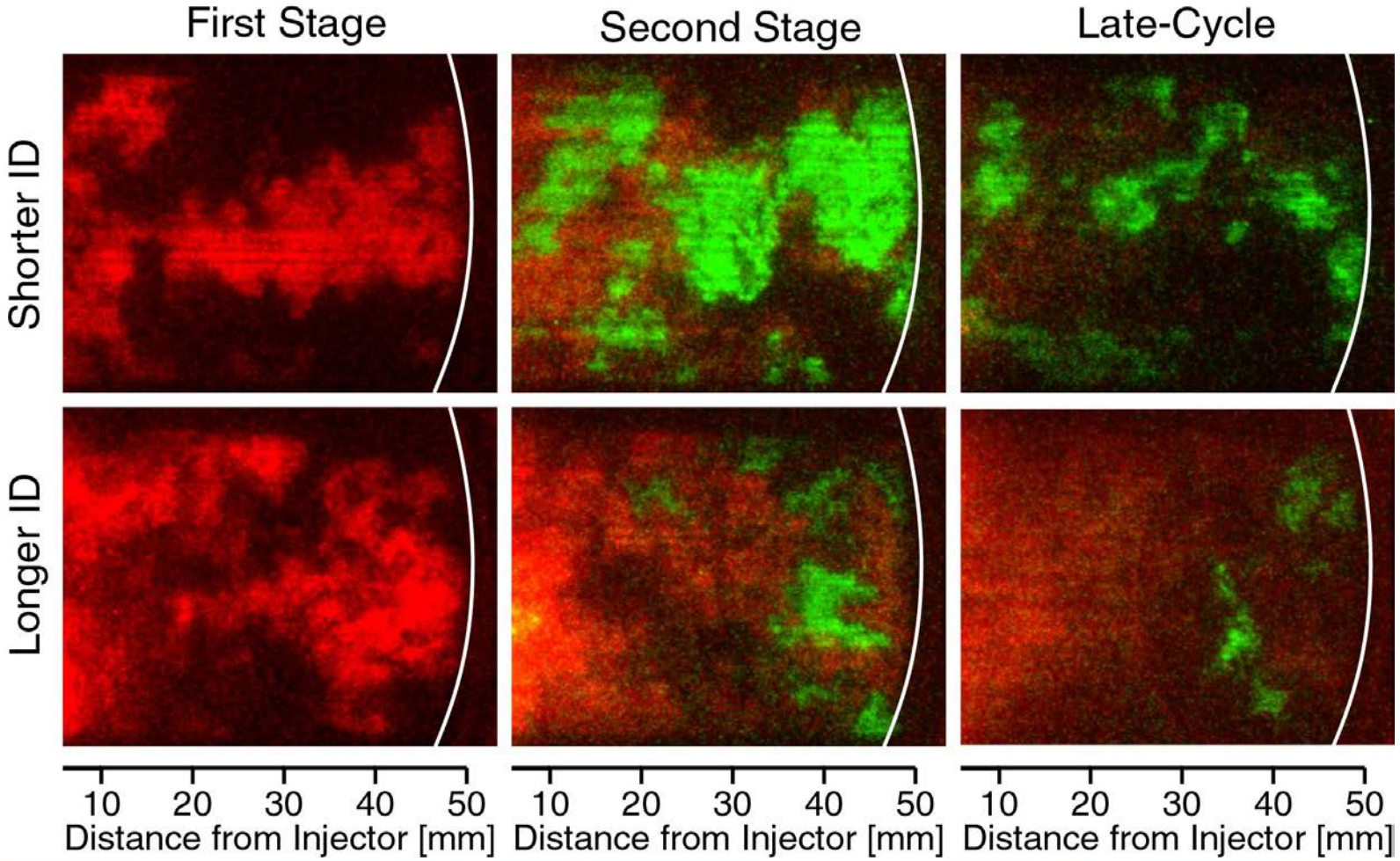
For longer LTC ignition dwell, formaldehyde PLIF shows UHC remains near injector late in the cycle

Red = Formaldehyde (H_2CO) fluorescence, Green = OH Fluorescence

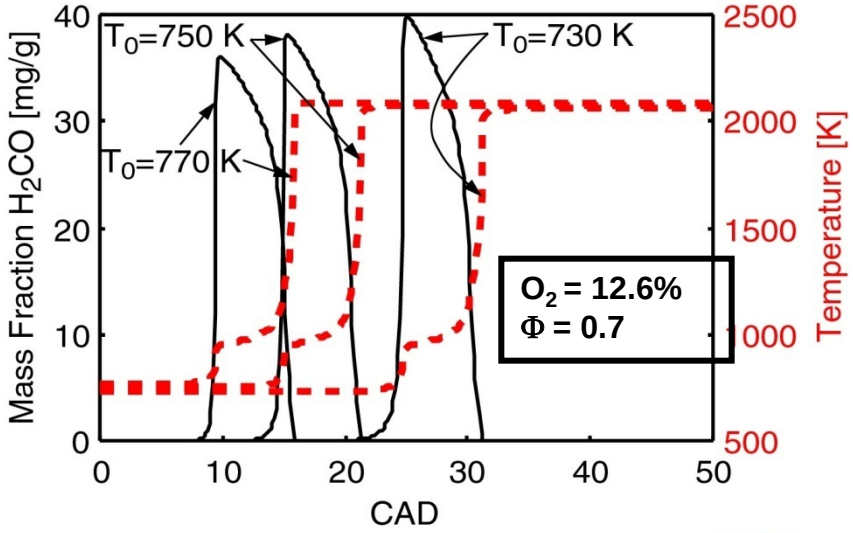
For Shorter ID, OH appears as H_2CO & UHC near injector are consumed

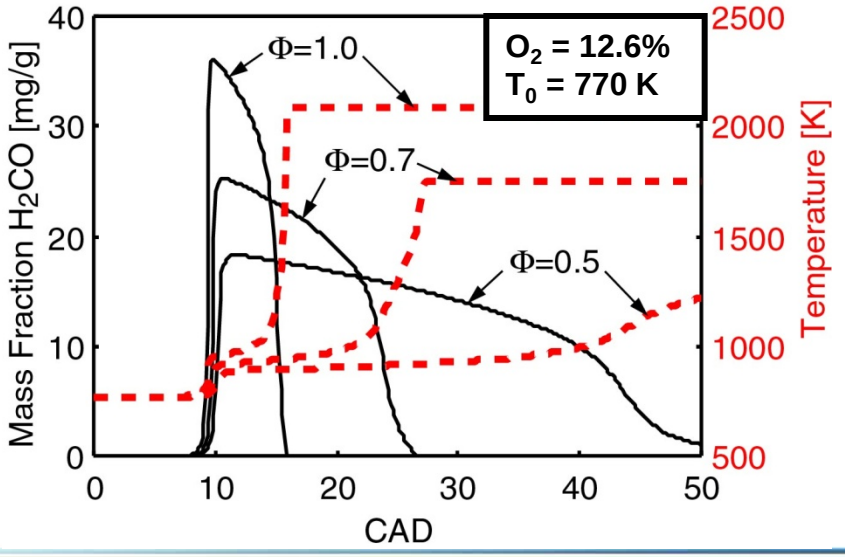
For Longer ID, H_2CO & UHC remain late in the cycle, especially near injector

5th US Comb. Meeting, Western States Comb. Inst., March 25-28, 2007



0-D chemical kinetic modeling insight: If formaldehyde persists, region is likely fuel-lean



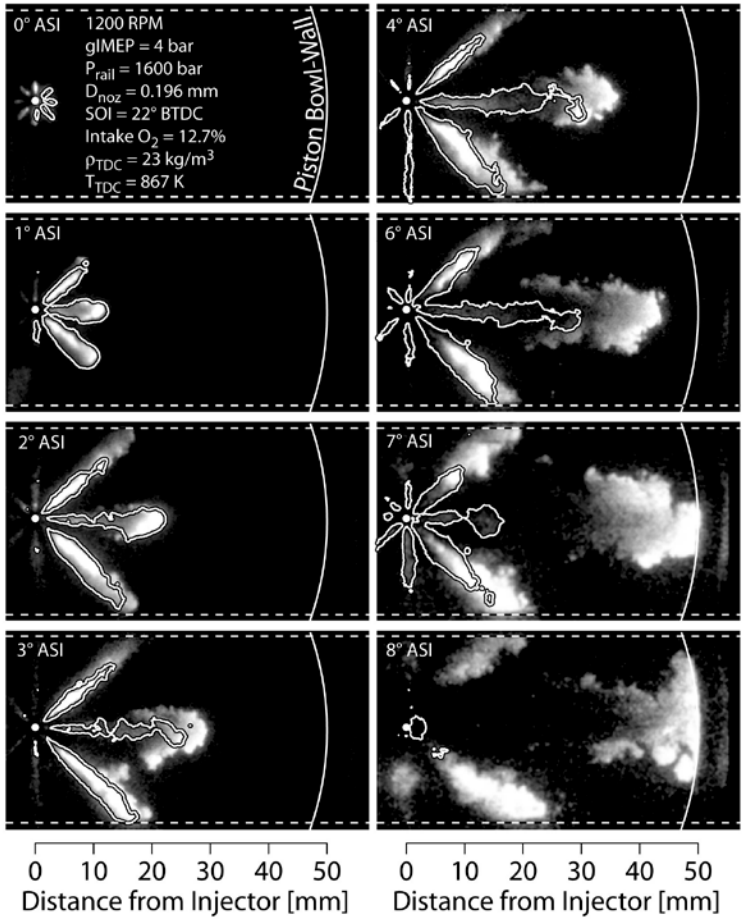


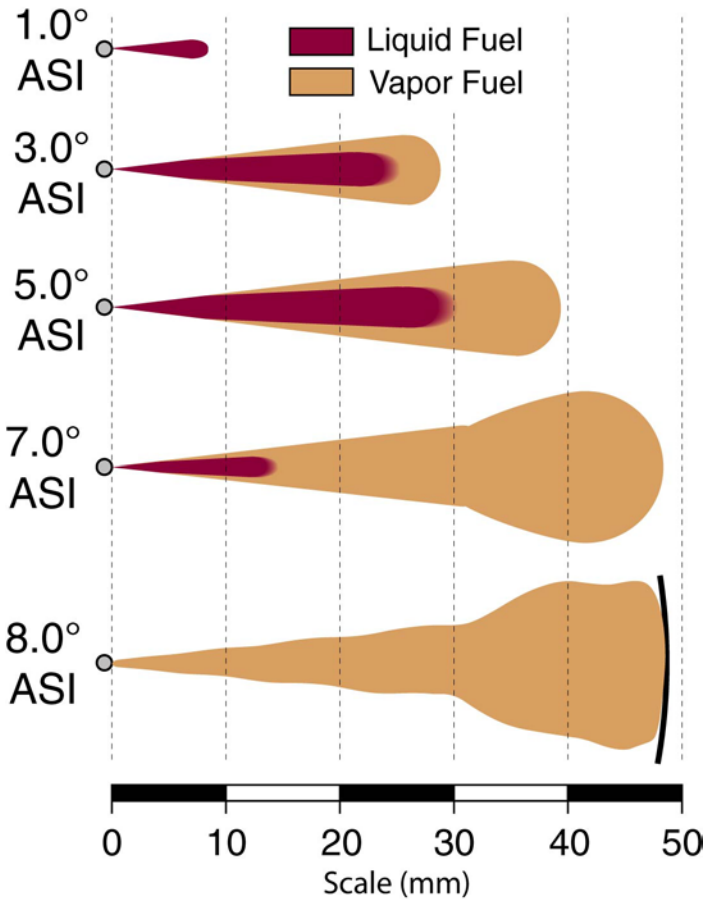
- Q: Is late formaldehyde caused by
  (1) low temperatures or
  (2) lean mixtures?
- (1): As temperature is decreased, H_2CO appearance is delayed, but residence time is constant.
- (2): As equivalence ratio is decreased, H_2CO time of appearance is constant, but residence time is increased.
- **Therefore, regions that have long-lasting, late-cycle H_2CO fluorescence are likely lean (near injector, after injection).**

Closed-reactor CHEMKIN simulations of n-heptane ignition using the Lawrence Livermore National Laboratories detailed mechanism of Curran, Pitz, and Westbrook

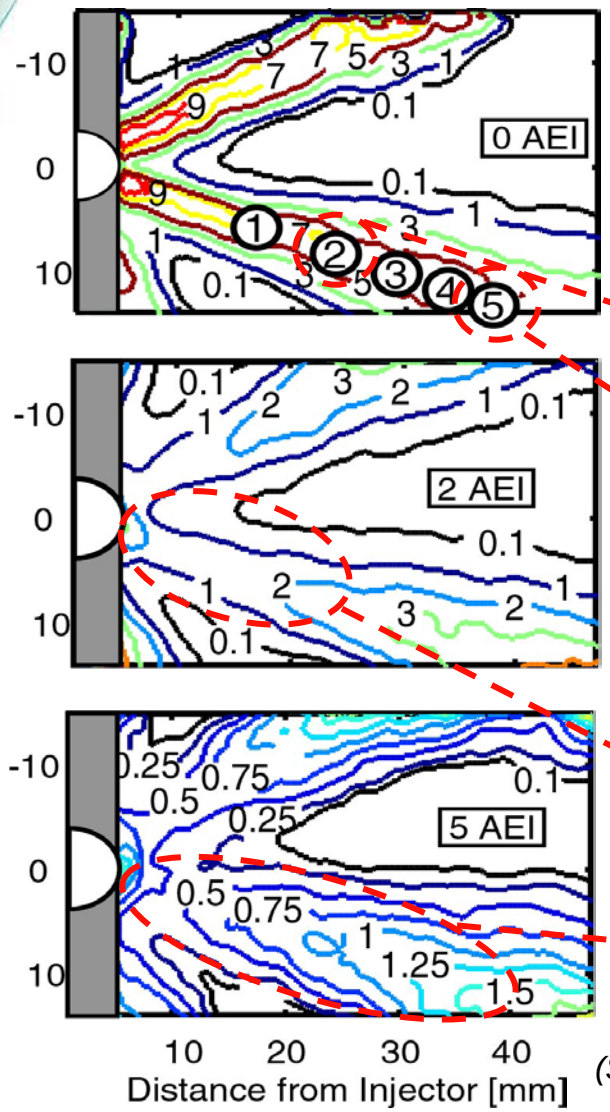
Liquid fuel “retreat” near end of injection also suggests fuel leaning after the end of injection

- Outline: Laser-Mie scatter off spray; Grayscale: fuel PLIF (w/ absorption)
- Liquid length recedes as injection ramps down – suggests fuel leaning





Fuel-tracer fluorescence shows near-injector mixtures rapidly become fuel-lean after EOI



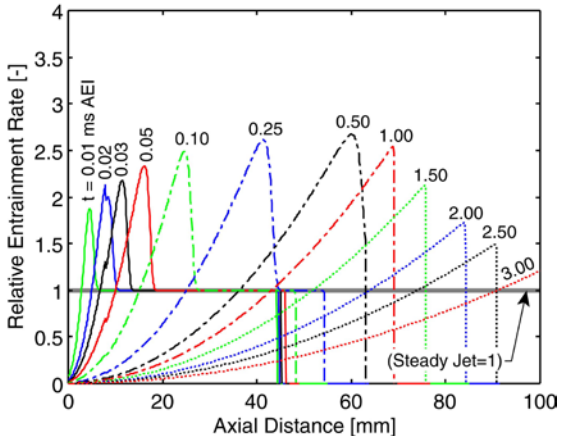
- At end of injection (0 AEI), mixtures are richer near injector (ϕ ~ 9) and leaner downstream
- In the quasi-steady jet, from a Lagrangian perspective (moving with jet fluid at penetration rate):
  - After 2° crank angle, 25 mm penetration to ϕ = 5 to 7
  - After 5° crank angle, 45 mm penetration to ϕ = 3 to 5
- After end of injection, mixtures near injector are much leaner than expected for downstream transport in a steady jet
  - At 2 AEI, within 25 mm penetration, ϕ = 1 to 3
  - At 5 AEI, within 45 mm penetration, ϕ = 0.5 - 1.5

(SAE 2007-01-0907, Musculus et al.)

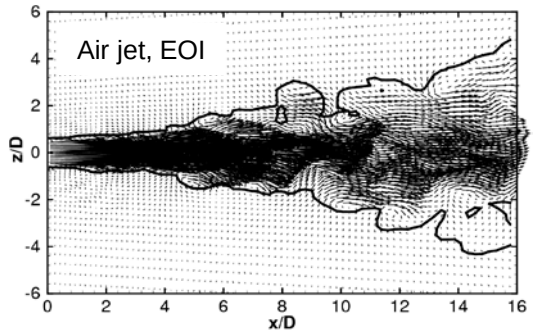
1-D analytic, KIVA RANS, and Sandia LES models predict wave of increased entrainment after EOI

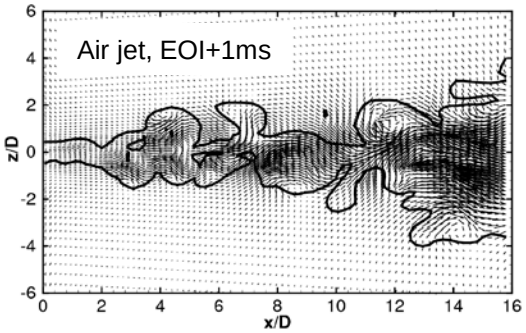
- 1-D model: Reduction in jet velocity draws in more entrainment, which reduces upstream velocity further, driving more entrainment, etc.
- LES: EOI ramp-down causes large flow structures to separate rather than collide; ambient fluid is entrained into gaps

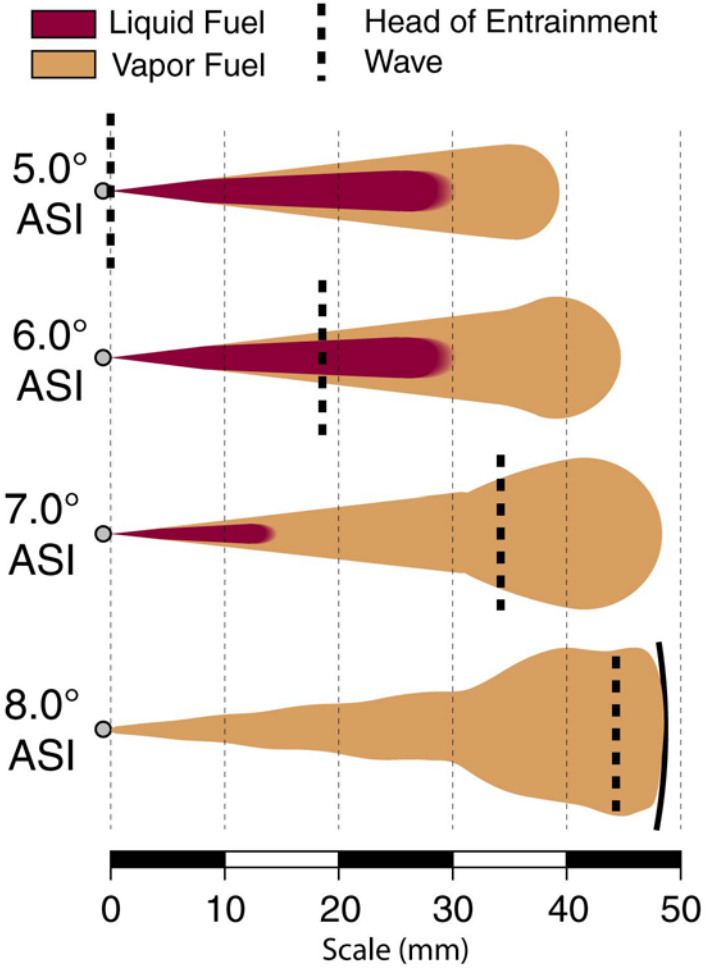
1-D model →



LES model ↓



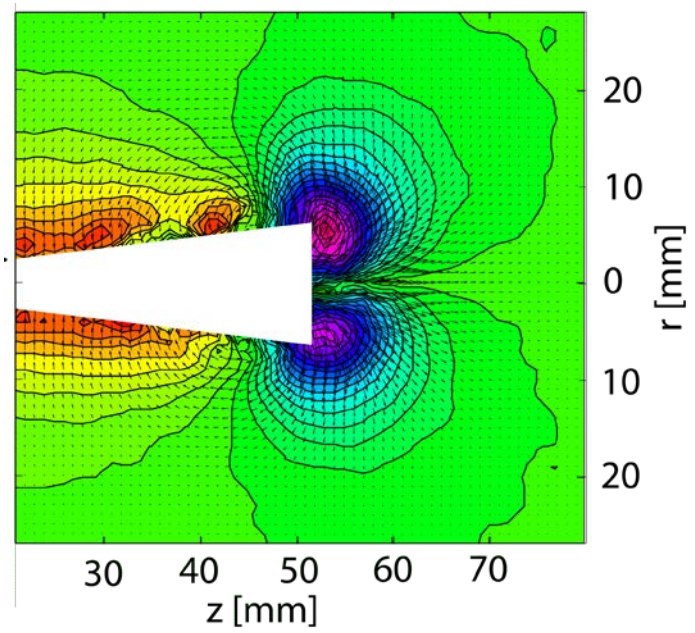


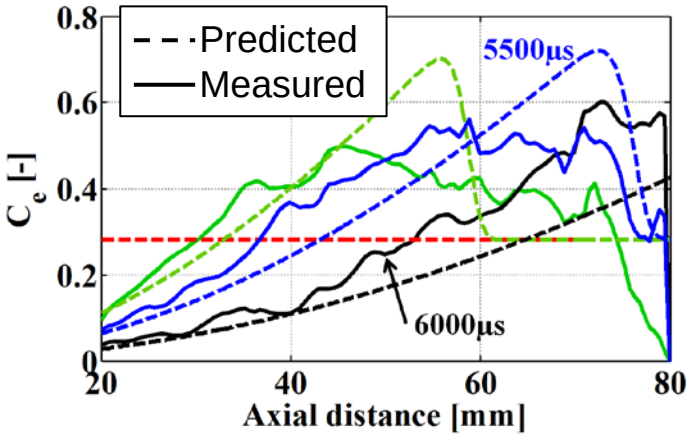


PIV data from Sandia/IFPEN ECN collaboration confirms end-of-injection mixing enhancements

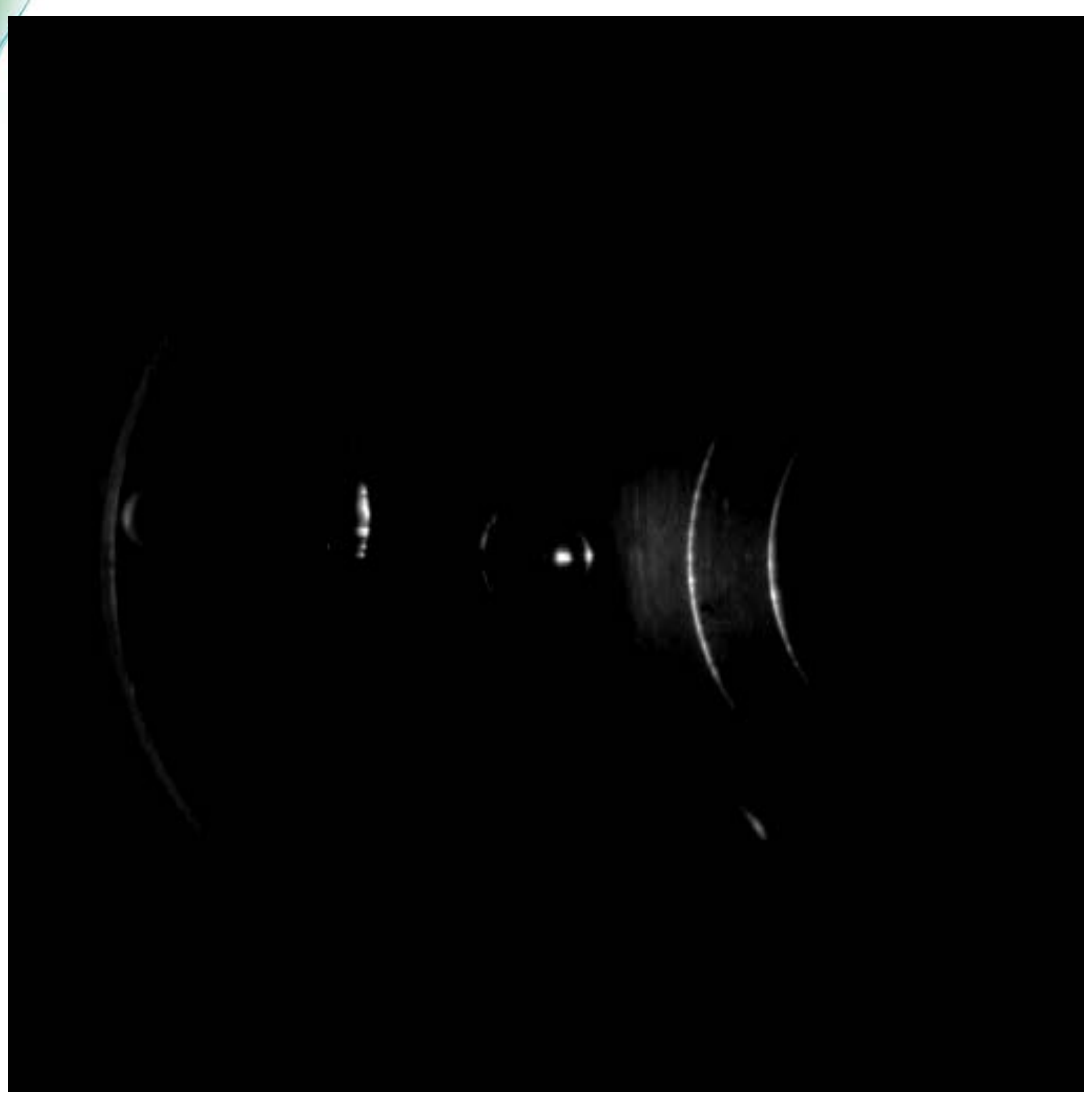
- From Engine Combustion Network (ECN): new high-quality particle image velocimetry (PIV) dataset
  - "Spray A" experiments conducted at IFPEN (Malbec & Bruneaux)
  - Entrainment analysis at Sandia
- Measured entrainment coefficient (C_e) agrees remarkably well with 1-D model
  - Small differences (confinement)

Great example of models providing new insight on an important physical effect later confirmed by experiments





Single-injection LTC condition: no combustion luminosity in center of chamber (UHCs)



Movie: Liquid Fuel + Combustion Luminosity

Single Injection

3 bar IMEP

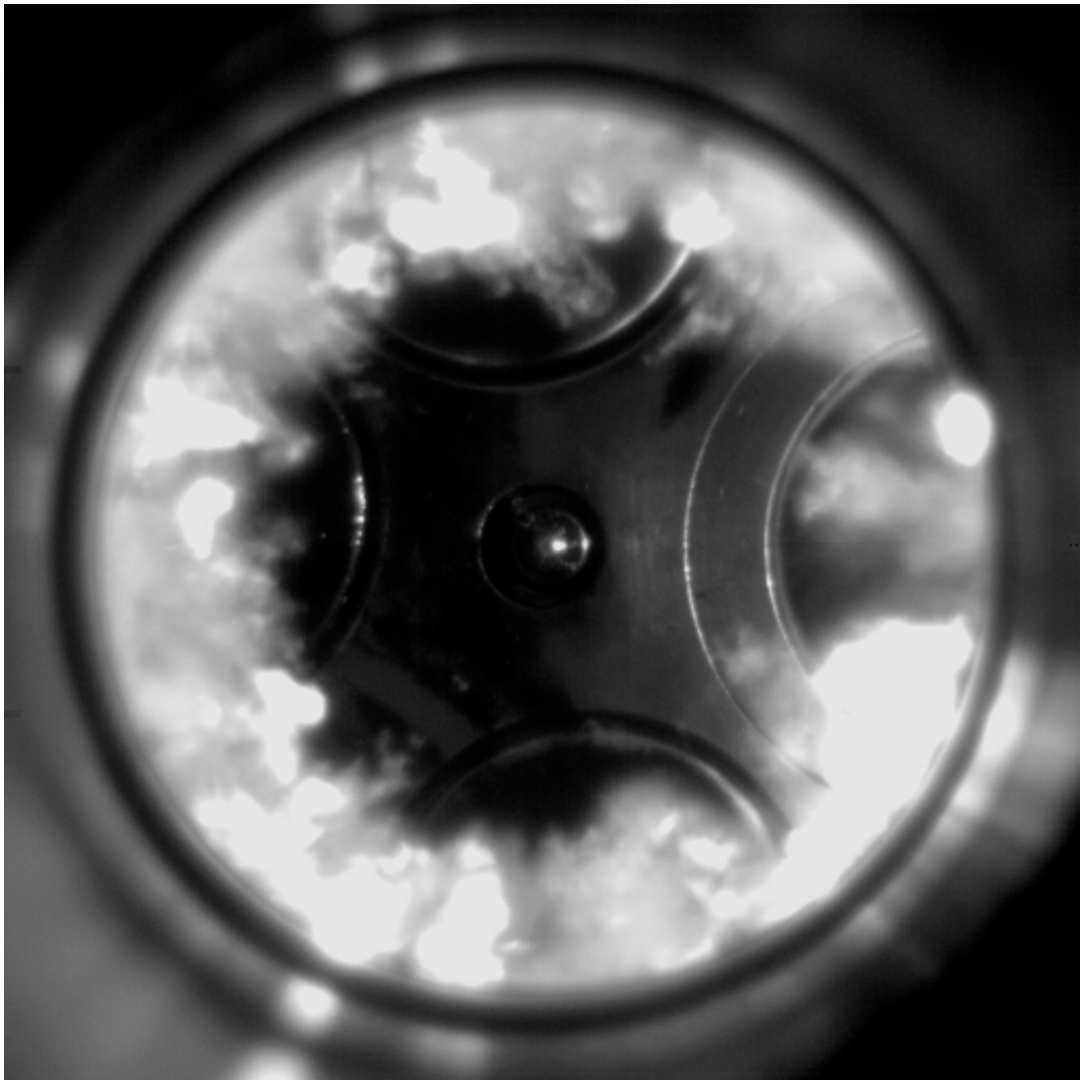
Fuel: CN 42.5 Diesel PRF (nC_{16} + iso-C_{16})

SOI: -5 ATDC

Intake O_2: 12.7%

- Previous laser diag. of similar condition show late-cycle UHC in center of chamber
  - No combustion luminosity in center of chamber

Single-injection LTC condition: no combustion luminosity in center of chamber (UHCs)



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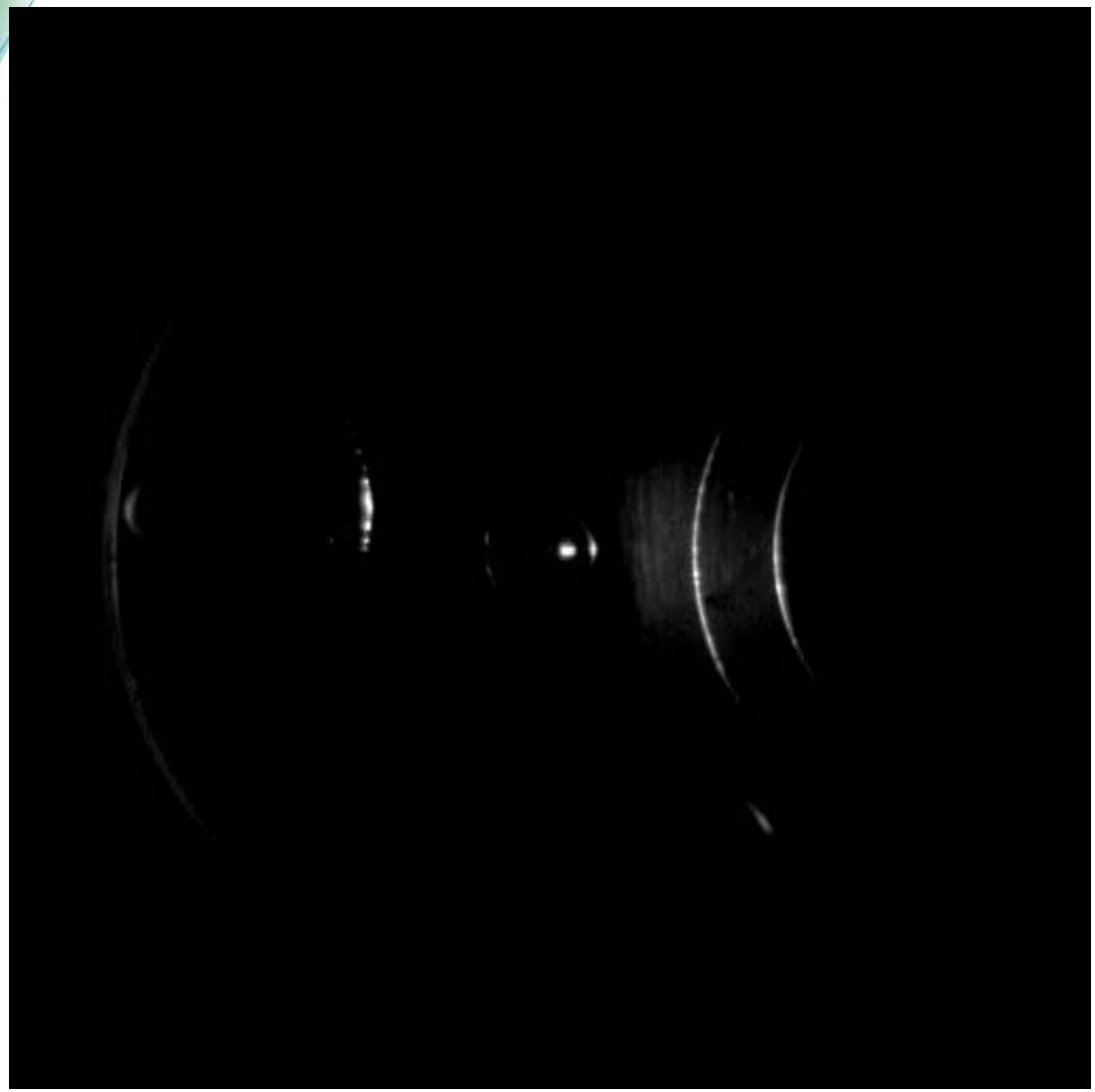
- Previous laser diag. of similar condition show late-cycle UHC in center of chamber
  - No combustion luminosity in center of chamber

Post-injection LTC condition: combustion luminosity appears in center of chamber



Movie: Liquid Fuel + Combustion Luminosity

Single+Post Injection

SOI: -5, +3 ATDC

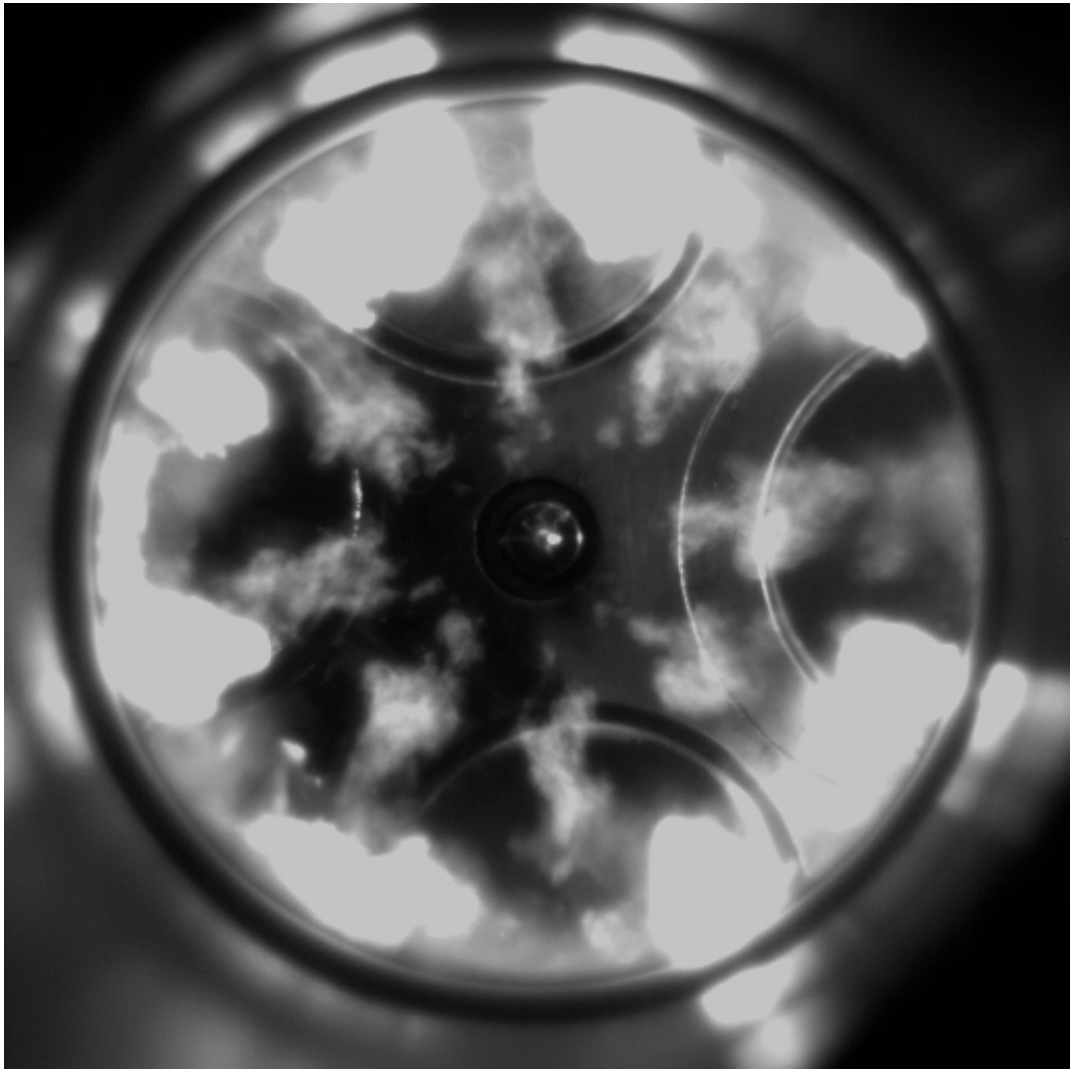
3 bar IMEP (same as single)

Fuel: CN 42.5 Diesel PRF (nC_{16} + iso-C_{16})

Intake O_2: 12.7%

- At same load, tiny post-injection decreases exhaust UHC by 15-25%
  - Strong combustion luminosity near center of chamber
  - UHC oxidation?

Post-injection LTC condition: combustion luminosity appears in center of chamber



Movie: Liquid Fuel + Combustion Luminosity

Single+Post Injection

SOI: -5, +3 ATDC

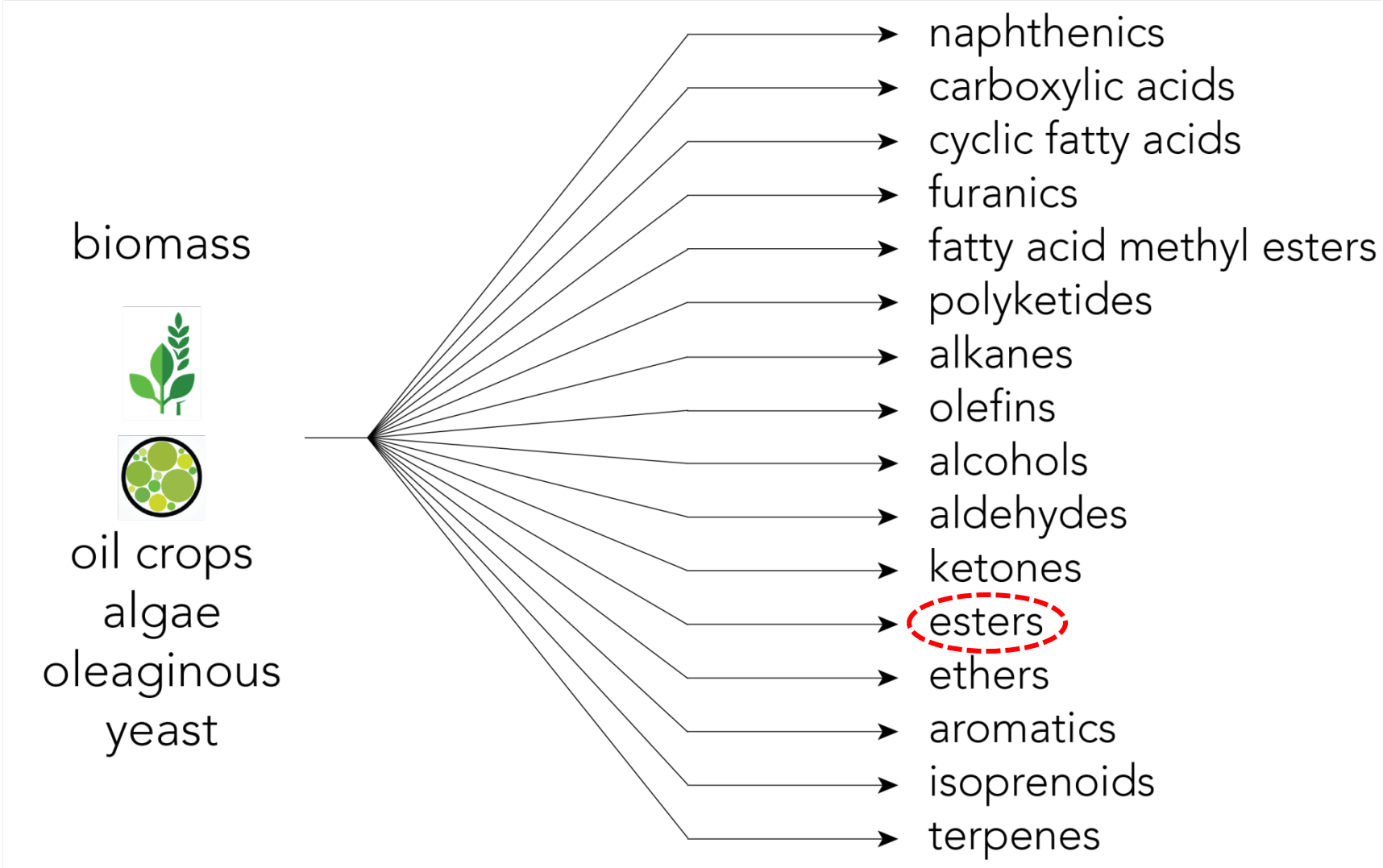
3 bar IMEP (same as single)

Fuel: CN 42.5 Diesel PRF (nC_{16} + iso-C_{16})

Intake O_2: 12.7%

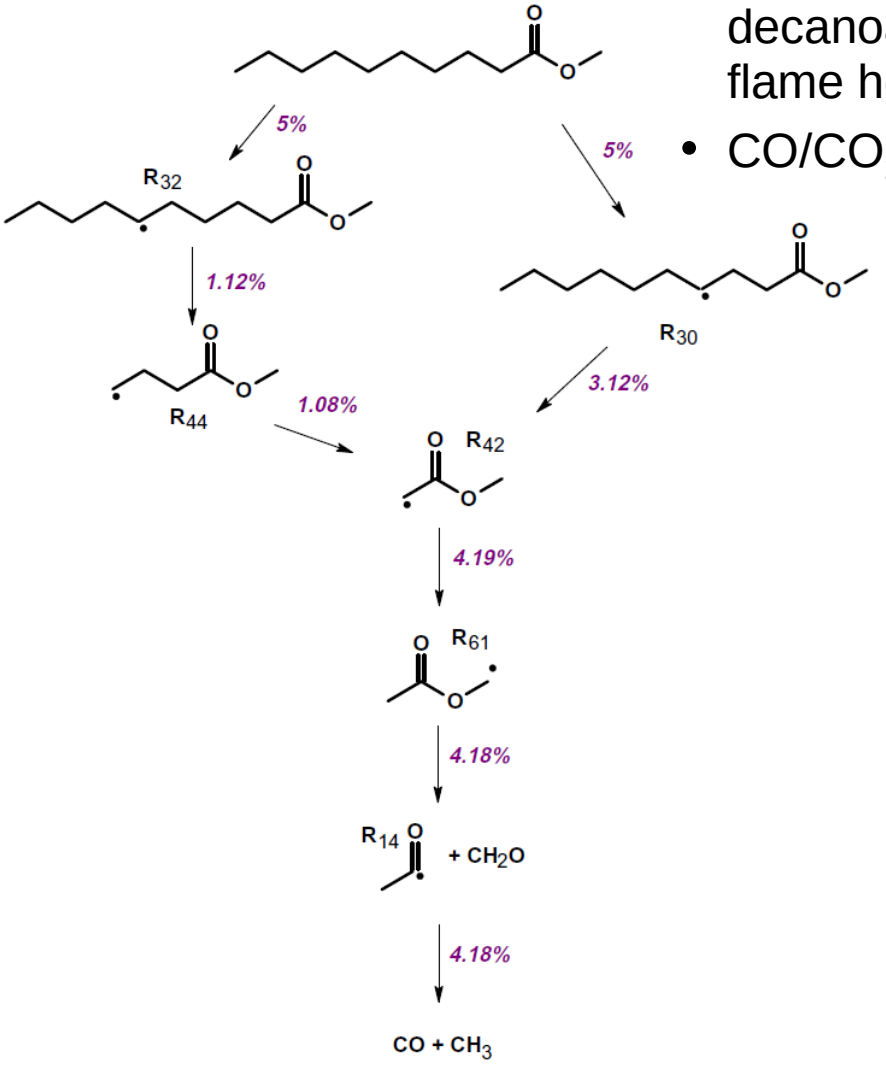
- At same load, tiny post-injection decreases exhaust UHC by 15-25%
  - Strong combustion luminosity near center of chamber
  - UHC oxidation?

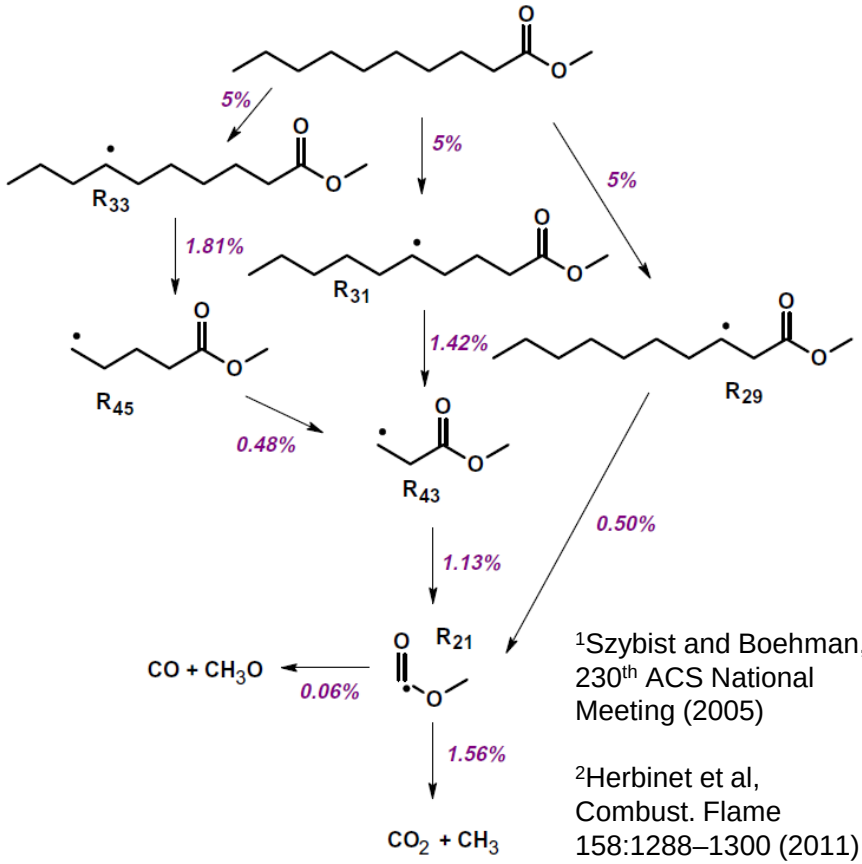
What opportunities are available for species detection to understand bio-fuel chemical kinetics?



Low-temperature reactions for large esters, e.g. methyl decanoate, produce early CO and CO_2

- Engine autoignition experiments: methyl decanoate produces much more CO_2 from cool-flame heat release than n-heptane[1]
- CO/CO_2 reaction pathways have been proposed [2]





[1]Szybist and Boehman, 230th ACS National Meeting (2005)

[2]Herbinet et al, Combust. Flame 158:1288–1300 (2011)

COMBUSTION RESEARCH FACILITY

Thank you!

COMBUSTION RESEARCH FACILITY

What Motivates the Development and Application of Laser/Optical Diagnostics for Diesel Engine Research?

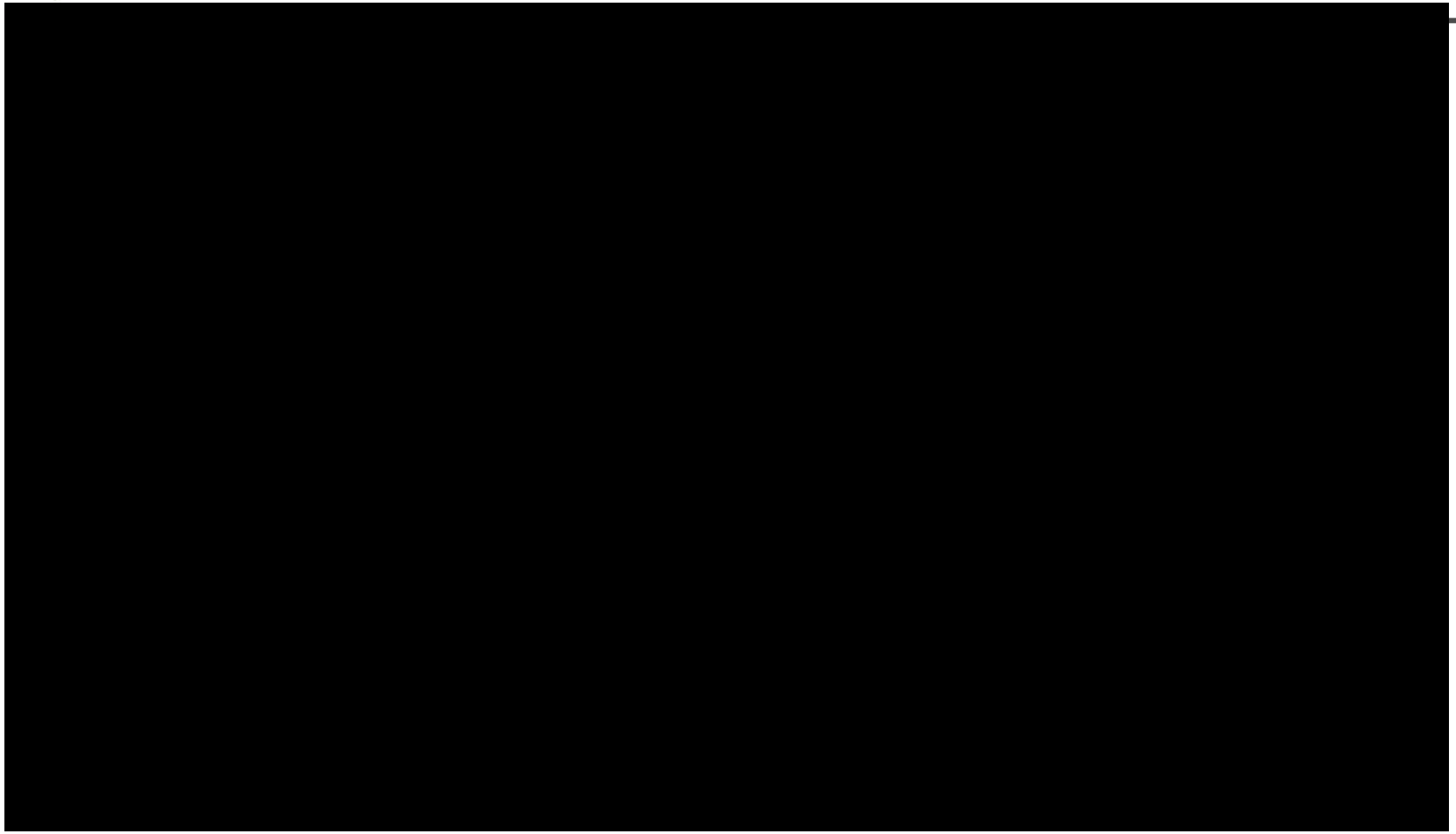
Mark P. B. Musculus
Sandia National Laboratories, USA

Lund University, Sweden

October 14, 2016

Sponsor: USDOE Office of FreedomCAR and Vehicle Technologies
Program Managers: Gurpreet Singh, Leo Breton, Kevin Stork

Diesel engines “rolling coal”

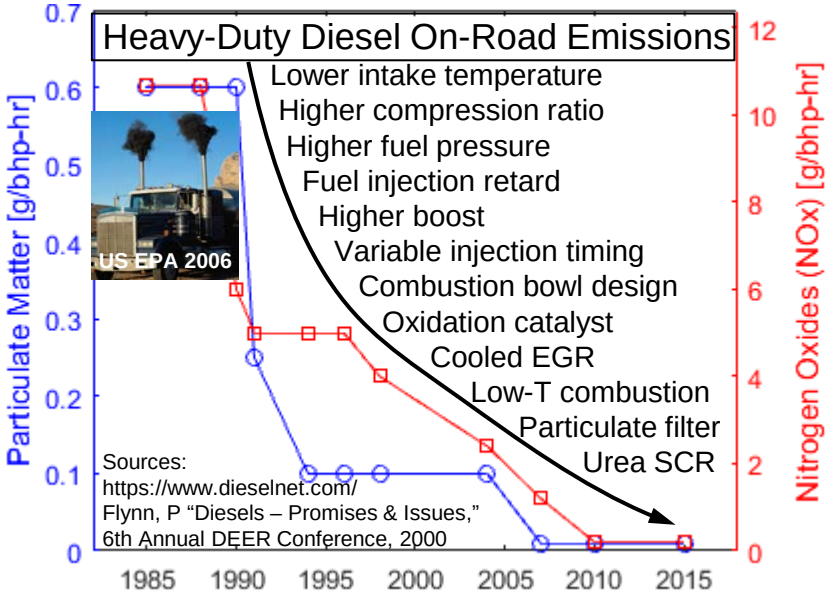


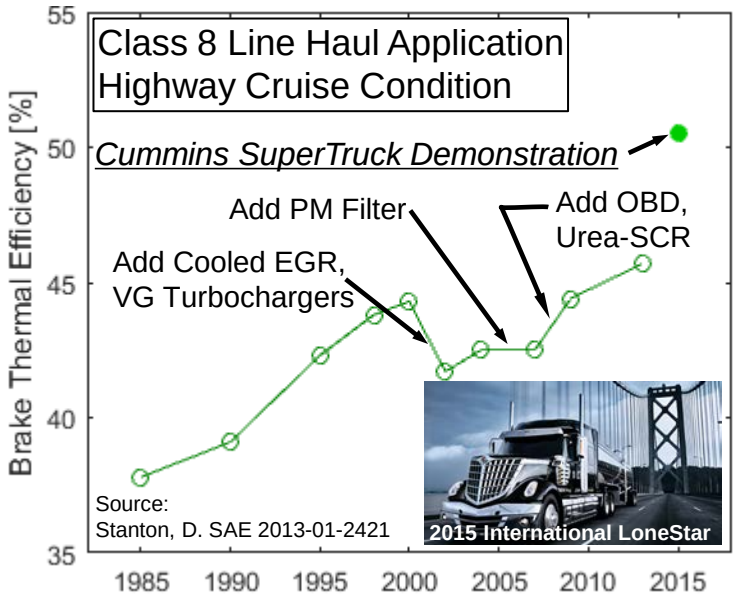
If efficiency/emissions don’t matter, and you only want max. power, then exceed the diesel “smoke point:” global equivalence ratio near ϕ=0-7-0.8

Stoichiometric air/fuel ratio=15:1, $\phi=(A/F_{stoich})/(A/F)$, so smoke at A/F<~20

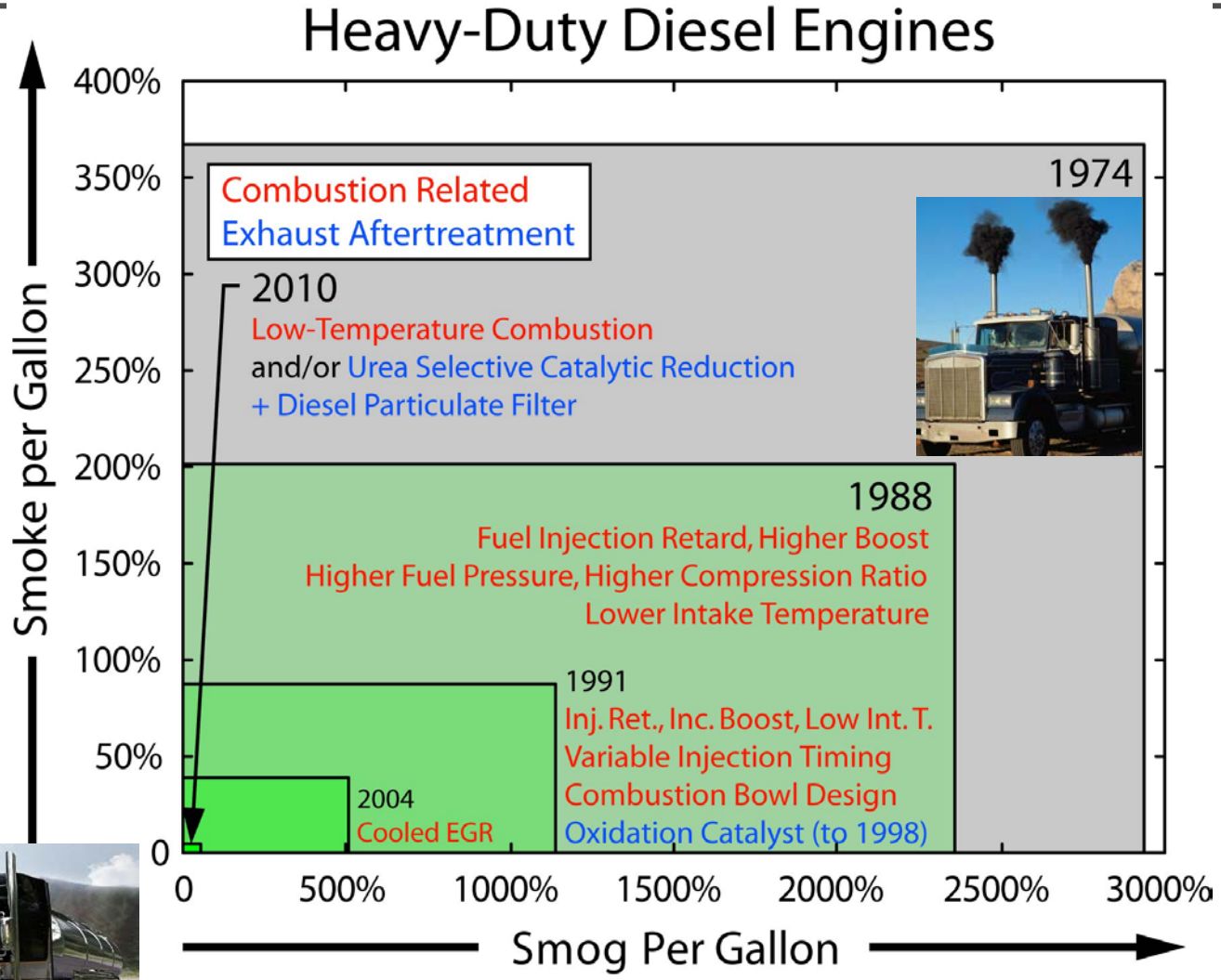
1985-2015: US Heavy-duty diesel emissions decreased over 50-fold, efficiency up by 8(13)% pts

- Because of its overall fuel-lean charge (λ>1.4 or ϕ<0.7), a conventional diesel engine cannot use the 3-way catalyst for exhaust aftertreatement that has worked well for stoichiometric gasoline engines since 1981
  - Needed to find in-cylinder solutions as emissions targets were tightened through 2004, then add aftertreatment in 2007/2010 (PM filter + Urea SCR)
- Some emissions reduction technologies also brought fuel efficiency improvements
  - DOE SuperTruck 2015 goal/demonstration: 50+% BTE; was <38% in 1985

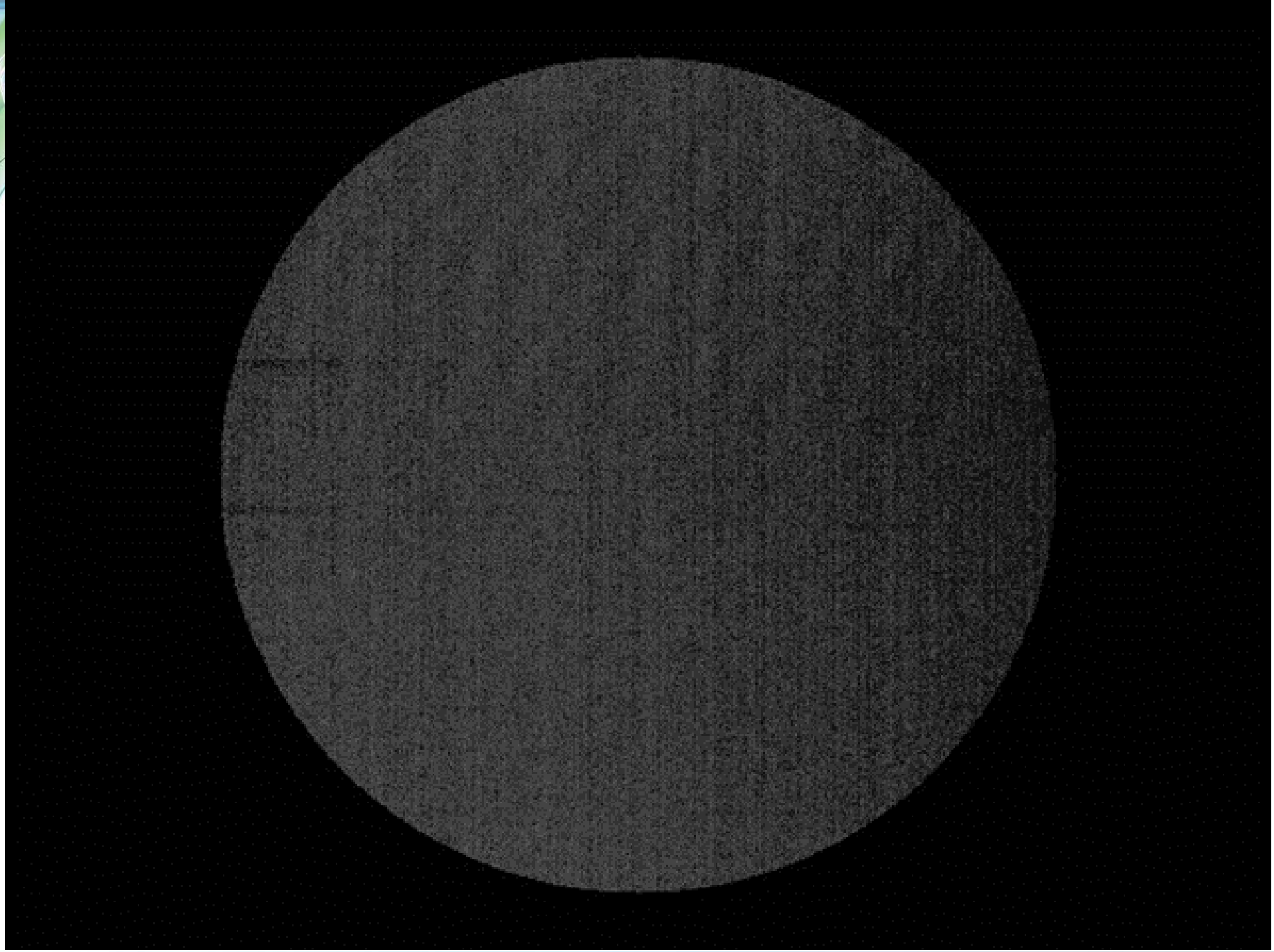




What if each resident of the tri-valley burned one gallon of diesel fuel per day in the year ... ?



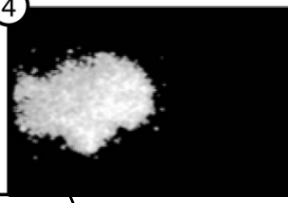
For more info, see Majewski WA and Khair MK, *Diesel emissions and their control*, Chapter 14, SAE International, Warrendale, PA (2006)

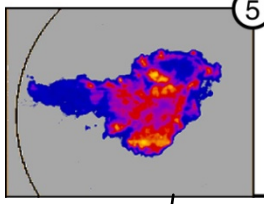


In-cylinder strategies to improve diesel emissions & efficiency were guided by optical diagnostics

O_2 = 21% (no EGR)
SOI = 10 BTDC
P_{inj} = 1000 Bar

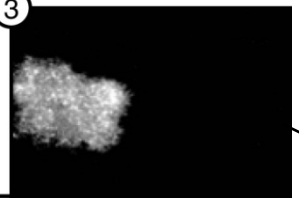
PAH PLIF: Soot Precursors
As hot ignition reactions increase the temperature in the jet, fuel fragments are formed into chemical building blocks for soot.



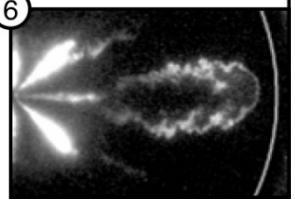


LII: Soot Concentration
Shortly after the premixed fuel burns, soot is formed in the hot, fuel-rich region throughout the jet cross-section.

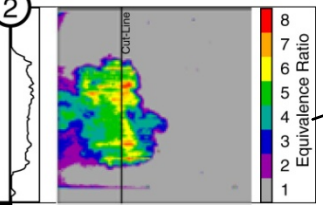
Chemiluminescence: Ignition
Spontaneous ignition reactions occur in the hot mixture of fuel and air throughout the leading portions of the jet.

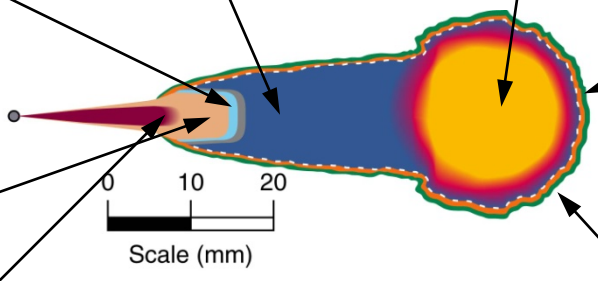


OH PLIF: Diffusion Flame
Shortly after the premixed fuel burns, a thin diffusion flame forms on the jet periphery, surrounding the interior soot cloud.

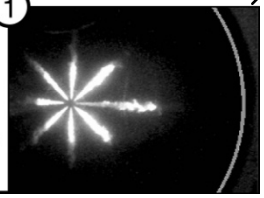


Rayleigh Scatter: Vapor Fuel
The vaporized fuel-air mixture downstream of the liquid is relatively uniform and fuel-rich (Φ = 2-4).

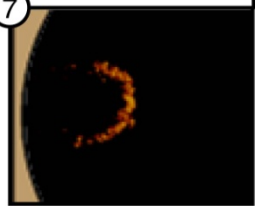




Mie Scatter: Liquid Fuel
After penetrating approx. 25 mm, the hot, entrained gases completely vaporize the liquid fuel.



NO PLIF: Thermal NO
NO forms on the periphery of the jet in the hot diffusion-flame products.

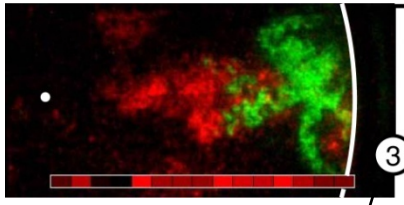


Liquid Fuel
Rich Vapor-Fuel/Air Mixture
Diffusion Flame
Fuel-Rich Premixed Flame
Initial Soot Formation
Thermal NO Production Zone
Soot Oxidation Zone
Low — High
Soot Concentration

Source: SAE 970873, Dec (1997)

We need new optical tools for new engines. Example: Low-temperature diesel combustion

O_2 = 13% (high EGR)
SOI = 22 BTDC
P_{inj} = 1200 Bar

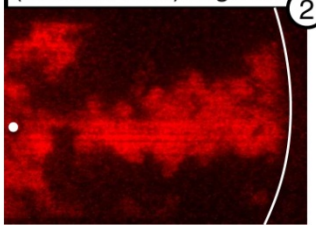


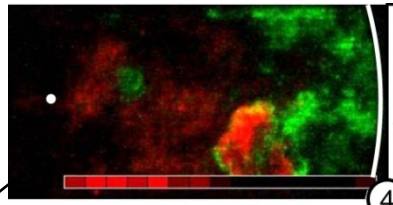
OH PLIF: 2nd-Stage Ignition
OH (green) appears downstream, in wide bands distributed over the width of the jet. Formaldehyde (red) remains upstream.

3

H_2CO PLIF: 1st-Stage Ignition
Formadehyde appears nearly simultaneously in the jet, from fuel-lean (upstream) to fuel-rich (downstream) regions.

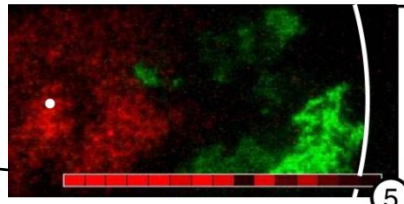
2





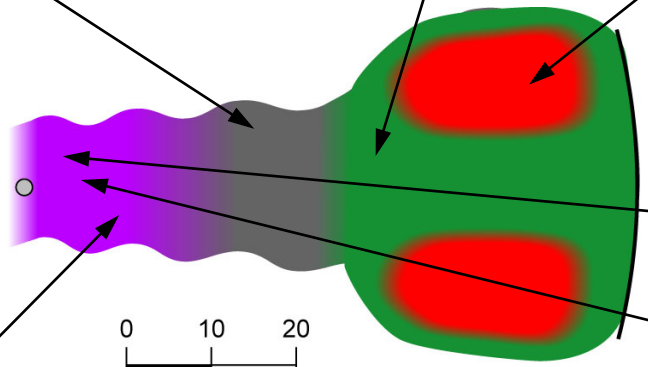
PAH PLIF: Soot Precursors
PAH species (bright red) form near the jet head-vortex, where adjacent jets interact. Formaldehyde (dim red) still remains, upstream.

4



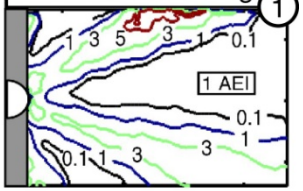
H_2CO PLIF: Unburned HCs
Late in the cycle, formaldehyde (red) indicates unburned hydrocarbons near the injector. OH (green) indicates combustion is more complete downstream.

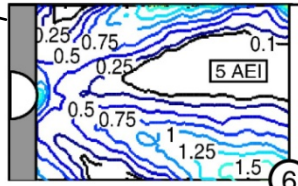
5



Fuel-Tracer PLIF: Φ
After fuel injection, equivalence ratios decrease and liquid fuel vaporizes rapidly due to faster mixing.

1





Fuel-Tracer PLIF: Φ
During ignition delay, near-injector mixtures become too fuel-lean to burn completely, leading to unburned HCs.

6

First-Stage Ignition
Second-Stage Combustion
Intermediate Ignition
PAH/Soot

Source: Prog. Energy Comb. Sci. 39:246-83, Musculus, Pickett, & Miles (2013)

Computer models are essential for engine design, but they required detailed knowledge of in-cylinder processes

- Cummins 2007 ISB diesel engine developed entirely by computer simulation
  - Experimental validation testing only after the low-emissions engine was built
- To develop new computer models for cleaner, more efficient engines, the science-base of combustion fundamentals is essential, and optical diagnostics are the primary tools to provide that science-base

Backup Slides

From biomass to bio-blendstocks: 9 Thrust I classes

- **Identified 9 molecular classes suitable for further evaluation in Thrust I (SI) engines**
  - Paraffins (especially highly branched paraffins), olefins, cycloalkanes, aromatics, alcohols, furans, ketones, ethers, and esters
- **Developed list of candidates from these classes based on:**
  - Open literature sources
  - Ongoing national laboratory research
  - Proposed plausible pathways from biomass to spark ignition blendstocks
- **Constructed tiered screening process using efficiency merit function, including expected optimal values for properties**

$$Merit = \frac{(RON_{mix} - 92)}{1.6} - K\frac{(S_{mix} - 10)}{1.6} + \frac{0.01[ON/kJ/kg](HoV_{mix} - 415[kJ/kg])}{1.6} + \frac{(HoV_{mix} - 415[kJ/kg])}{130} + \frac{(S_{Lmix} - 46[cm/s])}{3} - LFV_{150} - H(PMI - 2.0)[0.67 + 0.5(PMI - 2.0)]$$

47 bio-blendstocks pass high-level Tier 1 screening

Alcohols
Ethanol (reference only)
Methanol
n-Propanol
2-Propanol
1-Butanol
2-Butanol
2-Methylpropan-1-ol (isobutanol)
2-Methylbutanol
2-Methyl-3-buten-2-ol
2-Pentanol
Guerbet alcohols

Alkanes
Isooctane
2,2,3-trimethyl-butane (triptane)

Alkenes
Isooctene (2,4,4-trimethyl-1-pentene)

Aromatics
1,3,5-trimethylbenzene (mesitylene)
Vertifuel (60%+ aromatics)
Fractional condensation of sugars + upgrading
Methanol-to-gasoline
Catalytic fast pyrolysis
Catalytic conversion of sugars

Esters
Acetic acid, methyl ester (methyl acetate)
Butanoic acid, methyl ester (methyl butyrate)
Pentanoic acid, methyl ester (methyl pentanoate)
2-Methylpropanoic acid, methyl ester
2-Methlybutanoic acid, methyl ester
Acetic acid, ethyl ester (ethyl acetate)
Butanoic acid, ethyl ester (ethyl butanoate)
2-Methylpropanoic acid, ethyl ester
Acetic acid, 1-methylethyl ester
Acetic acid, butyl ester (butyl acetate)
Acetic acid, 2-methylpropyl ester
Acetic acid, 3-methylbutyl ester
Anaerobic acid fermentation plus esterification mixture

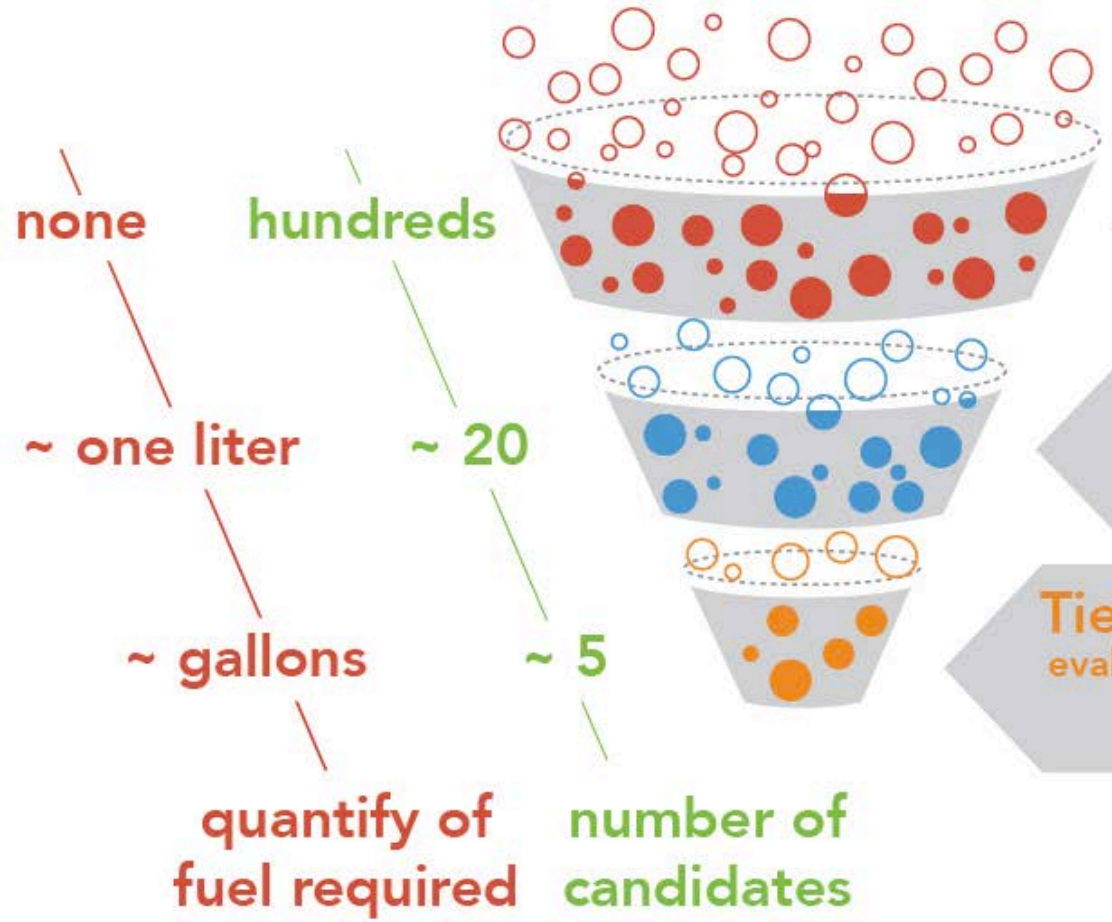
Ethers
Methoxybenzene (anisole)

Furans
2-Methylfuran
2,5-Dimethylfuran
40/60 Mixture of 2-methylfuran/2,5-dimethylfuran

Ketones
2-Propane (acetone)
2-Butane (methylethylketone; MEK)
2-Pentanone
3-Pentanone
Cyclopentanone
3-Hexanone
4-Methyl-2-pentanone (Methylisobutylketone)
2,4-Dimethyl-3-pentanone
3-Methyl-2-butanone

Multifunctional Mixtures
Methylated lignocellulosic bio-oil

Down-selection of bio-blendstocks progresses in 3 tiers



Tier 1: high-level screening

boiling point	corrosivity
freezing point	toxicity
solubility	heteroatom conc.
ignition quality	etc.

Tier 2: candidate selection

fuel merit function *	state of technology
life cycle GHG	infrastructure compatibility
land use, water	flash point, flammability
economics	etc.

Tier 3: candidate evaluation

evaluate promising candidates in engine tests