Recent Research Results from the Sandia Advanced Fuels Laboratory

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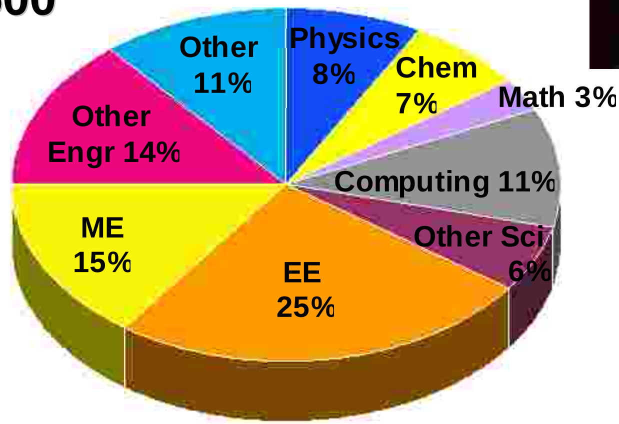
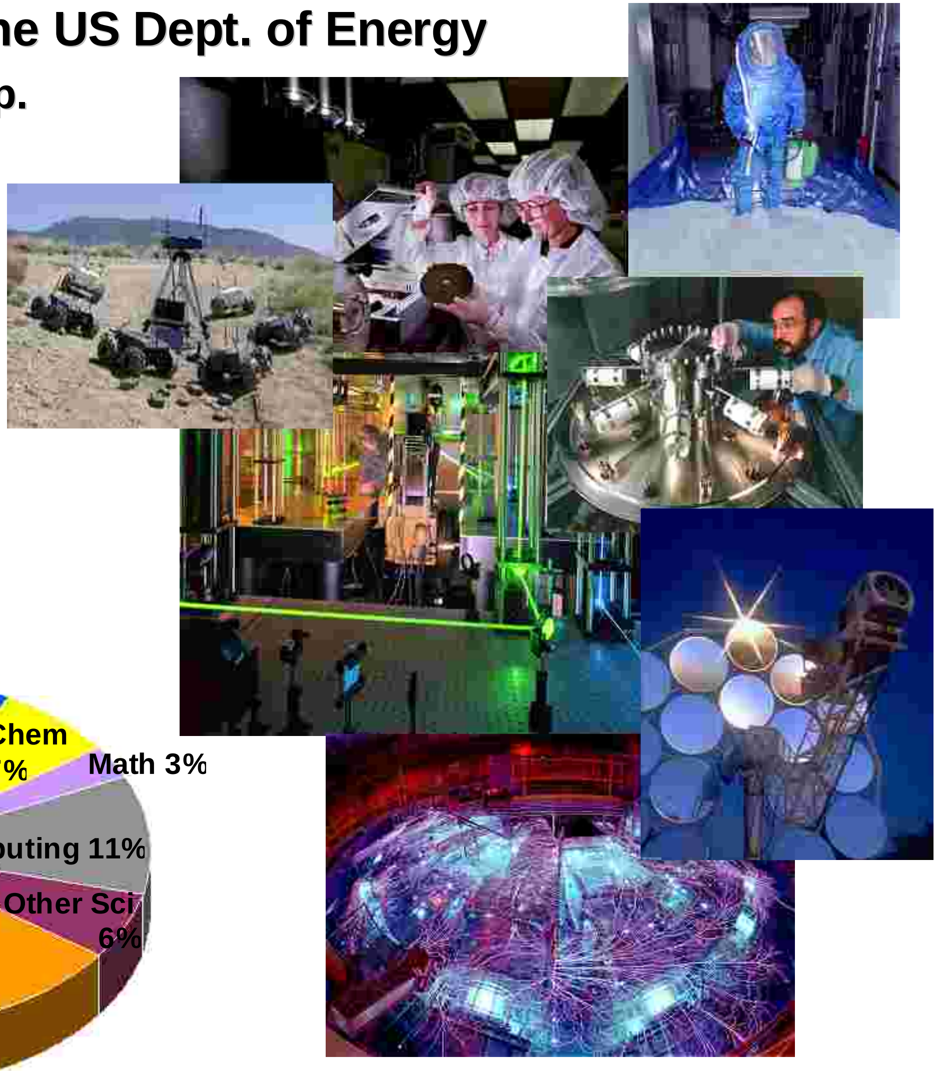
Presentation Outline

- **Overview of Sandia programs and facilities**
- **Sandia Advanced Fuels Laboratory**
- **Recent results**
  - ? **Dilute clean diesel combustion**
  - ? **Biodiesel NO_x increase**
- **Conclusions**
- *Additional recent results and references*

What is Sandia?

- A national laboratory funded by the US Dept. of Energy
  - ? Operated by Lockheed-Martin Corp.
- Technical programs include
  - ? Engineering Sciences
  - ? Computational and Information Sciences
  - ? Materials and Process Science
  - ? Pulsed Power Sciences
  - ? Microelectronics and Photonics Sciences
- Sandia has ~ 7500 employees
  - ? 2100 Masters
  - ? 1400 Ph.D.
  - ? Majority are engineers
  - ? 900 in CA





Sandia Has Facilities in Numerous Locations

Albuquerque, New Mexico

Tonopah Test Range, Nevada

WIPP, New Mexico

Livermore,California

Yucca Mountain, Nevada

Kauai Test Facility, Hawaii

Engine-Related Research at the CRF

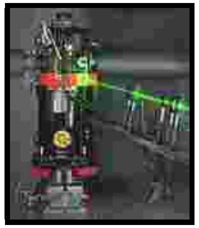
- **Engine Combustion Department has 7 laboratories (one principal investigator in each lab, dept. manager is Dennis Siebers)**

Constant-Volume Vessel
Lyle Pickett (PI)
Tim Williams (PD)

Fuel Effects
Chuck Mueller (PI)
Glen Martin (PD)
Krishna Lakshminarasimhan (PD)

HCCI Fundamentals
John Dec (PI)
Magnus Sjoberg (LTE)
Wontae Hwang (PD)

HCCI, Light-Duty
Richard Steeper (PI)
Russ Fitzgerald (PD)



HECC, Heavy-Duty Diesel
Mark Musculus (PI)

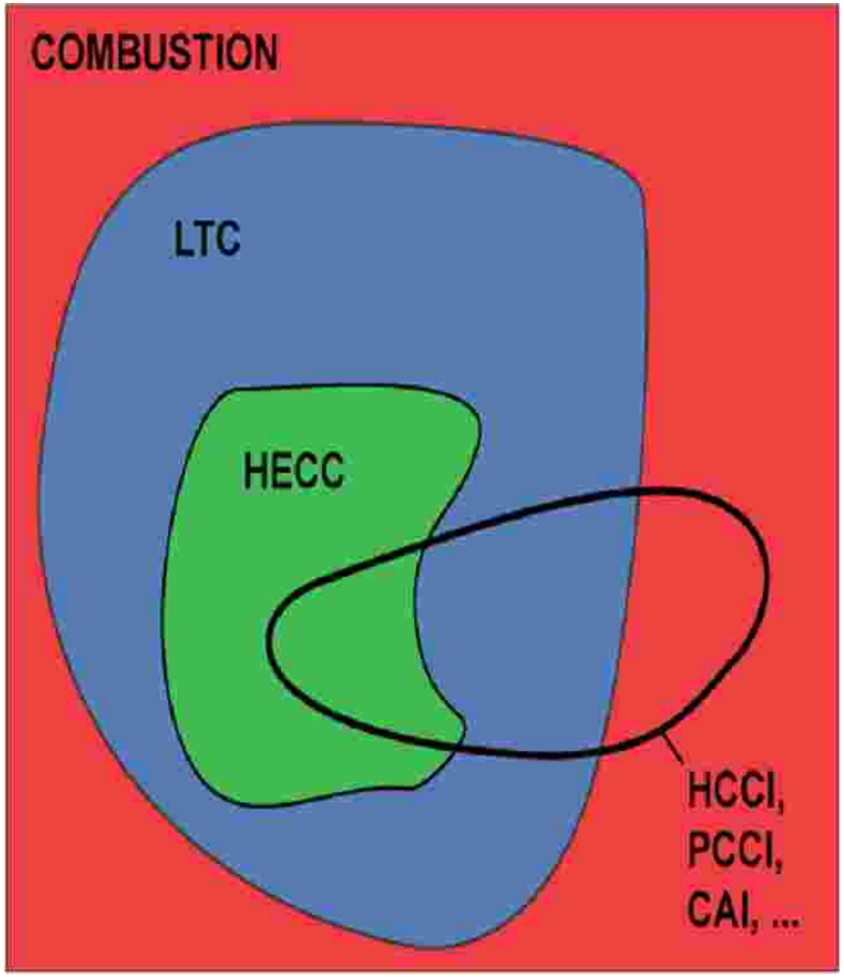
HECC, Light-Duty Diesel
Paul Miles (PI)
Will Colban (PD)
Isaac Ekoto (PD)

HECC, Hydrogen
Sebastian Kaiser (PI)

Sandia Fuels Project Vision

High-efficiency, clean combustion (HECC) using advanced and/or non-petroleum fuels:

- **Robust operation**
- **Acceptable heat release**
- **High power density**



HECC = High-Efficiency, Clean Combustion

- *Efficiency similar to conventional diesel*
- *US 2010 heavy-duty regulations achieved with oxidation catalyst*

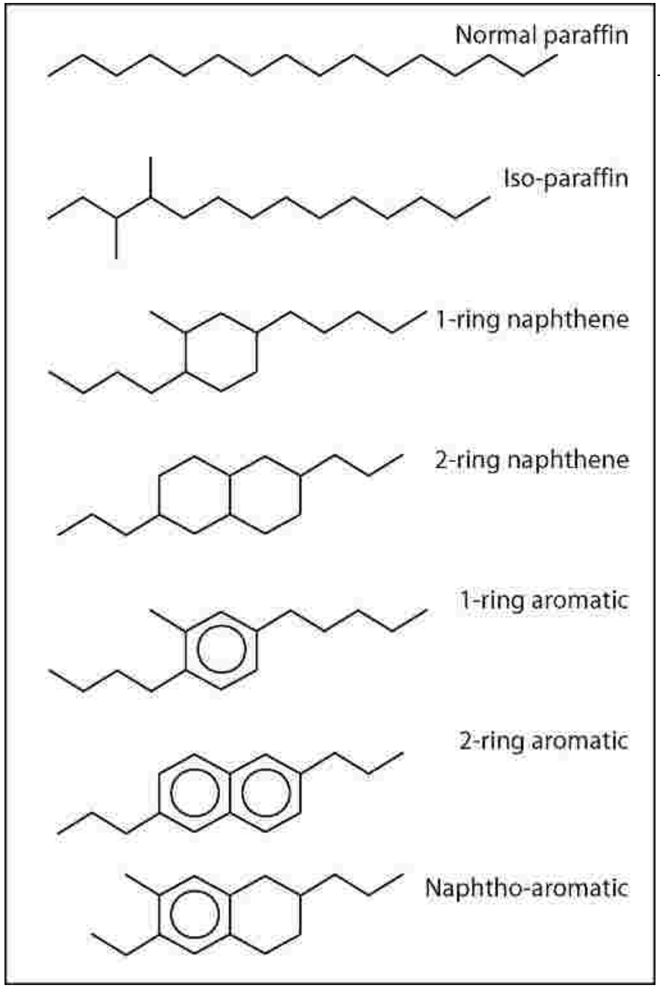
LTC = Low-Temperature Combustion

- *No constraints on efficiency*
- *Peak T low enough to minimize NO_x*

HCCI = Homogeneous Charge Compression Ignition

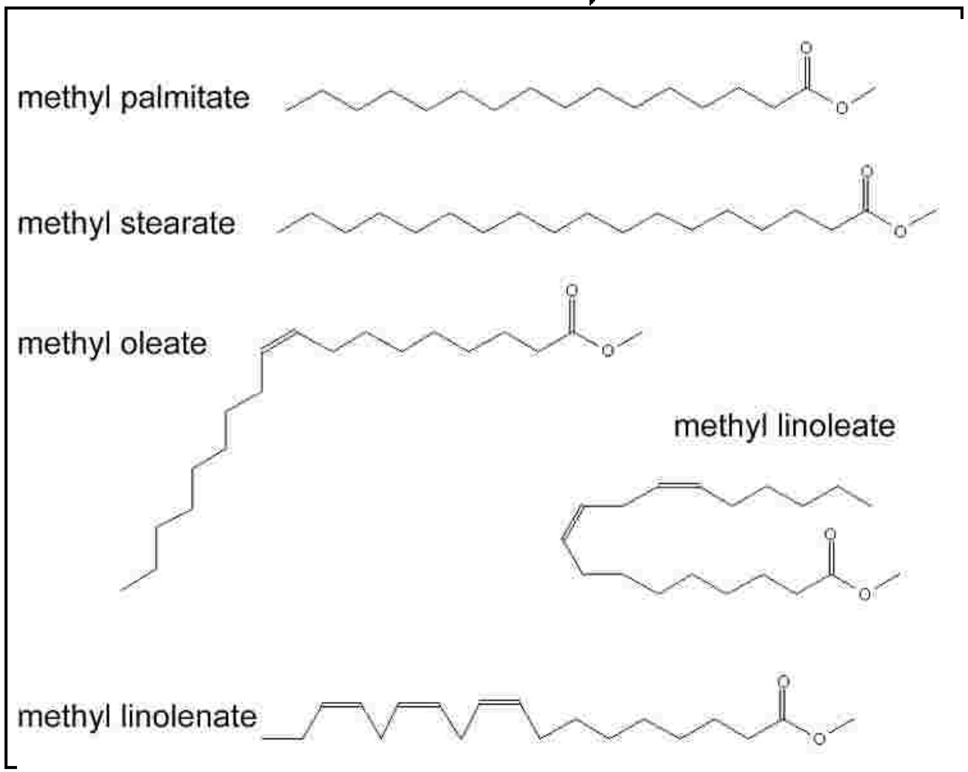
New Fuels Can Be Very Different from Conventional Fuels, and Burn Differently

Conventional diesel



from Farrell et al., SAE 2007-01-0201

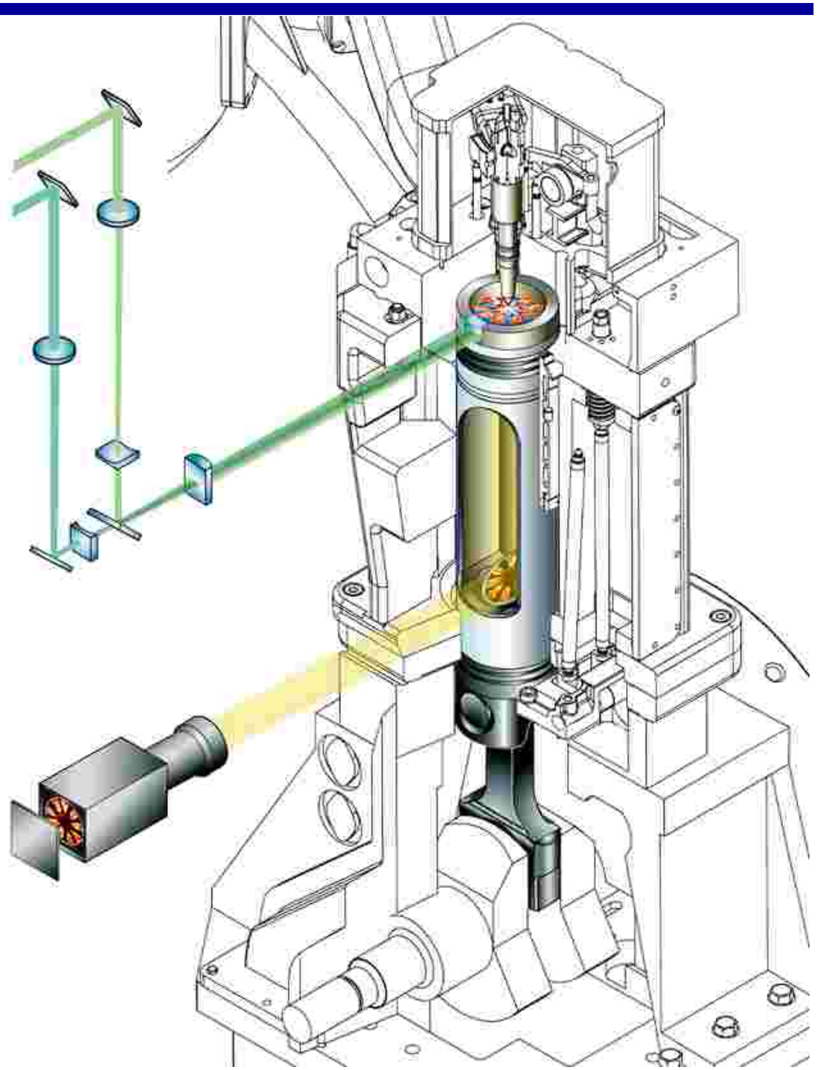
Biodiesel (soy methyl esters)



from Mueller, CRF News, May/June 2006

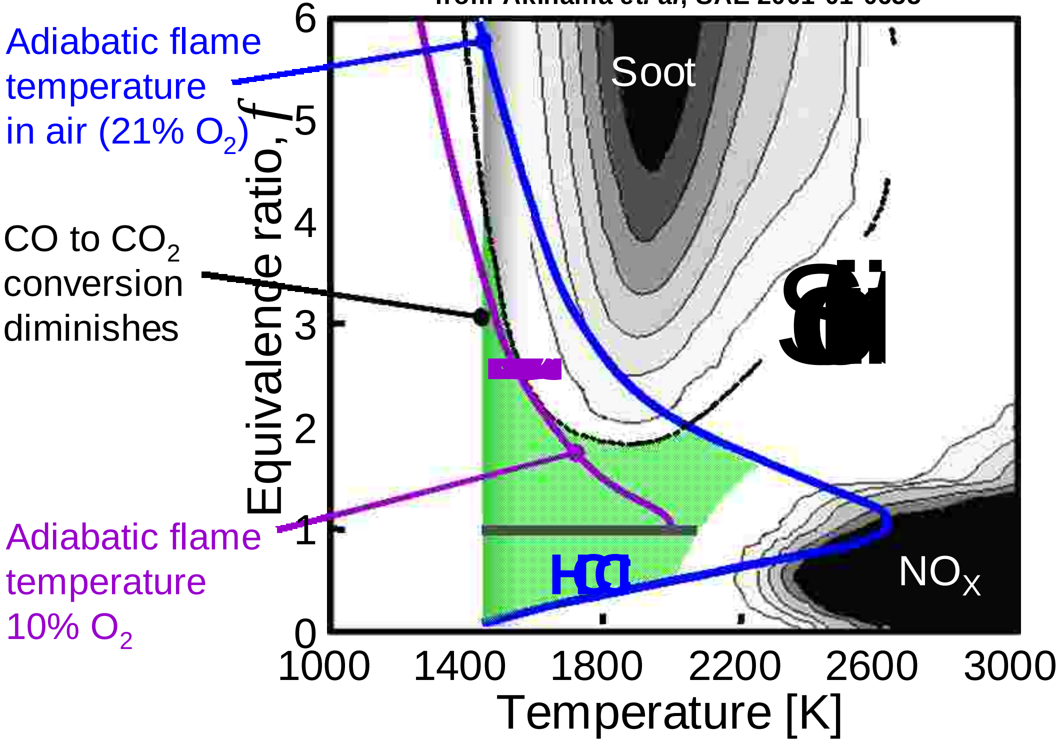
Optical Engine Specifications and Schematic

Research engine	**1-cyl. Cat 3176**
Cycle	**4-stroke CIDI**
Valves per cylinder	**4**
Bore	**125 mm**
Stroke	**140 mm**
Conn. rod length	**225 mm**
Conn. rod offset	**None**
Piston bowl diameter	**90 mm**
Piston bowl depth	**16.4 mm**
Squish height	**1.5 mm**
Swirl ratio	**0.59**
Displacement per cyl.	**1.72 liters**
Compression ratio	**11.3:1**
Simulated compr. ratio	**16.0:1**



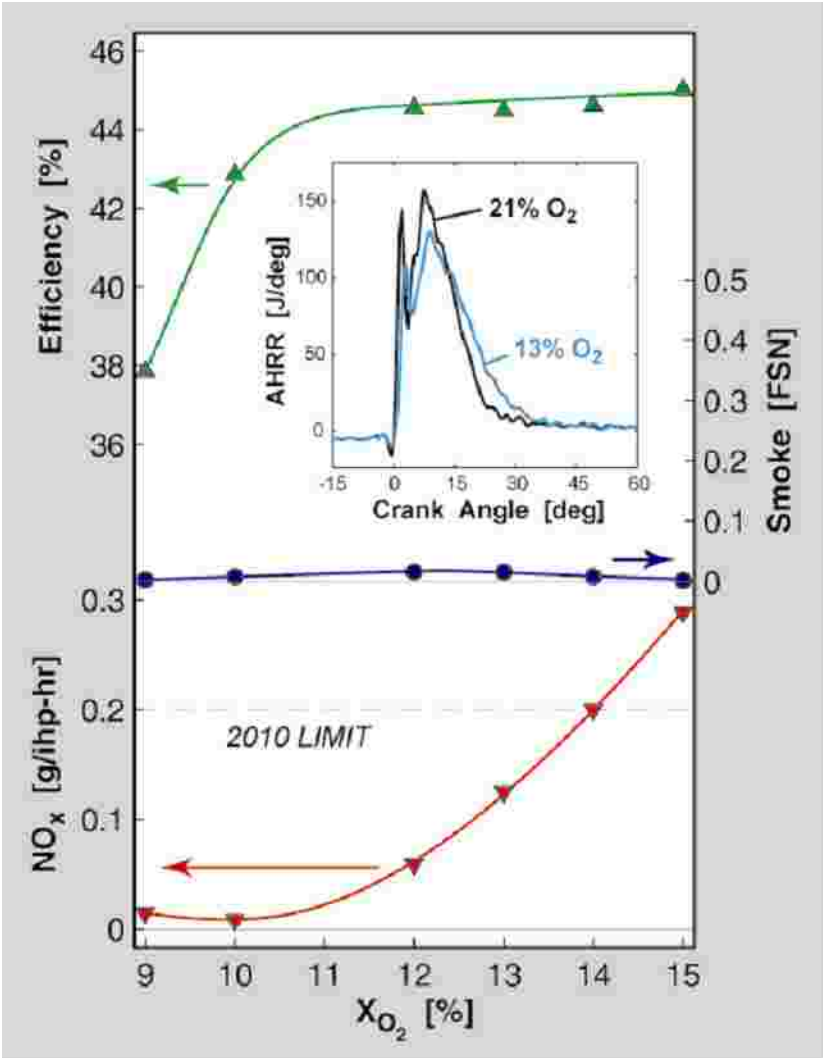
Quartz windows in piston and upper periphery of cylinder liner enable optical access

Dilute Clean Diesel Combustion (DCDC) Using Oxygenated and Emerging Fuels

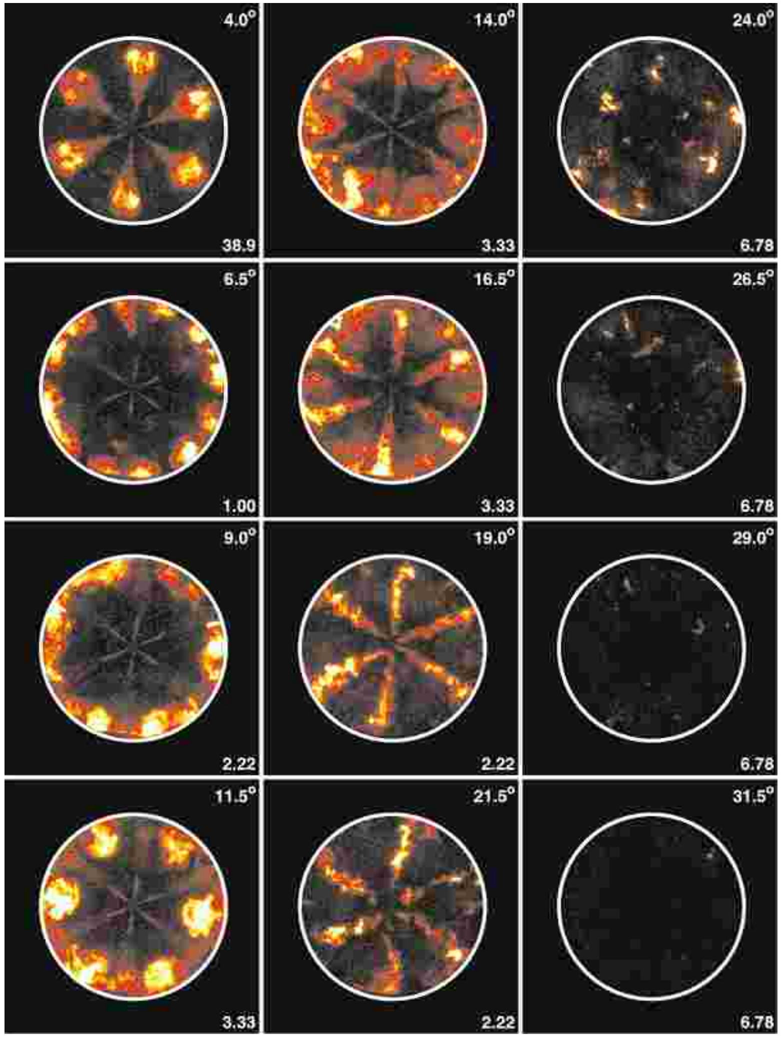


DCDC Simultaneously Achieves Low Emissions and High Efficiency

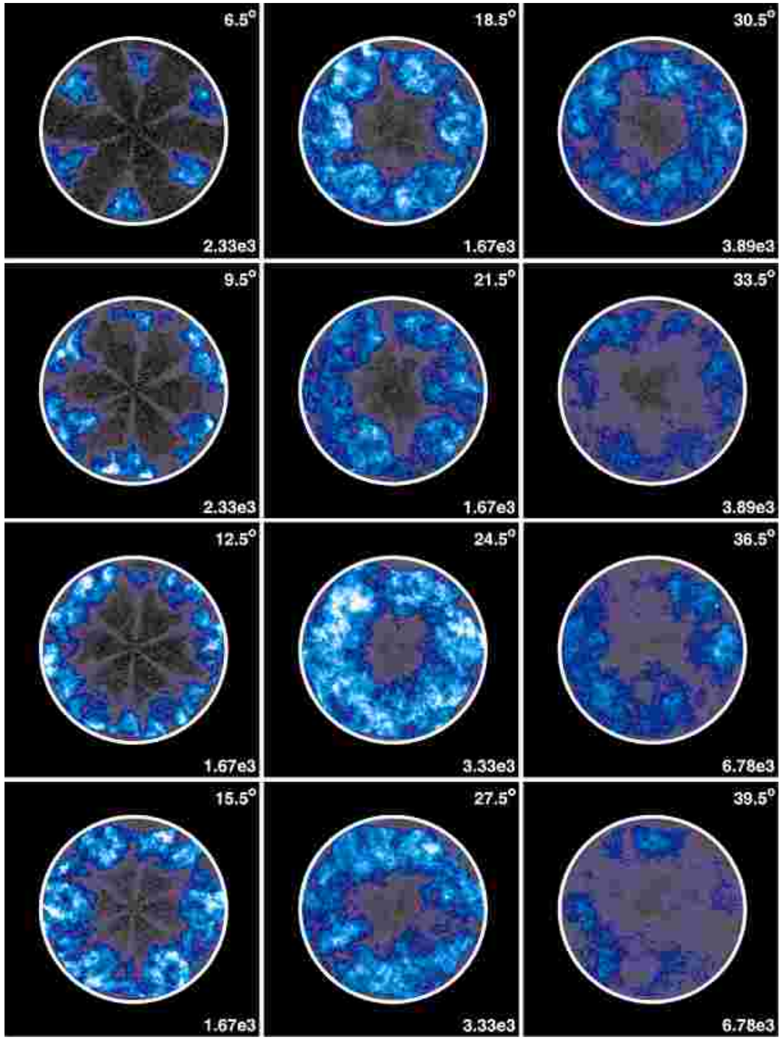
- **Operating conditions**
  - ? Diethylene glycol diethyl ether (DGE) fuel
  - ? 1200 rpm, 7-bar IMEP
  - ? Steady-state operation
  - ? -9 ° C, 1.4 bar intake
  - ? EGR simulated by N_2 dilution
- **High-load operation also demonstrated in optical engine**
  - ? 18-bar IMEP (2/3 load)
  - ? 0.09 g/ihp-hr NO_x
  - ? 0.26 FSN smoke
  - ? Load and efficiency limited by peak cylinder pressure capability of optical engine



Natural Luminosity Imaging of Undiluted and Highly Dilute Combustion (DGE Fuel)



Undiluted



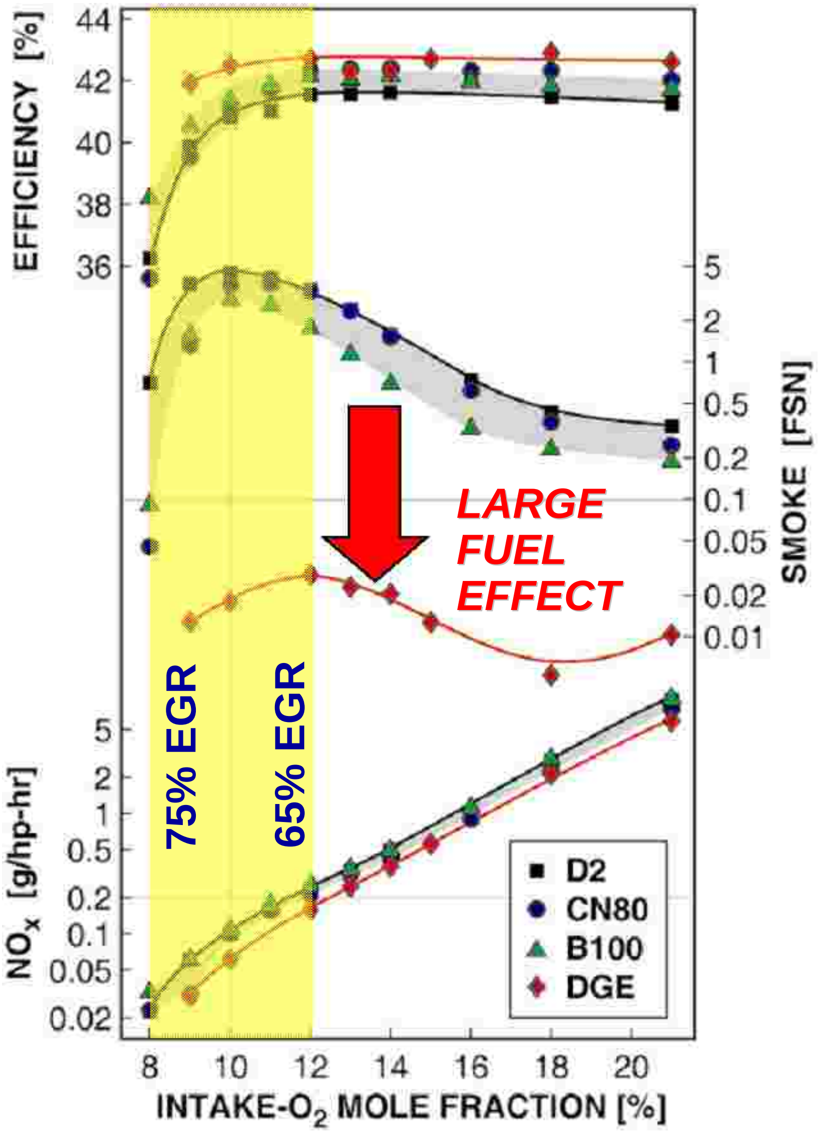
9% Intake-O_2 Mole Fraction

More-Conventional Fuels and Operating Conditions

- **Fuels**
  - ? **B100 = neat soy biodiesel (Peter Cremer Nexsol BD-0100)**
  - ? **CN80 = 80-cetane PRF blend, 76.5 vol% *n*-hexadecane + balance heptamethylnonane**
  - ? **D2 = Phillips #2 diesel reference fuel**
- **Operating conditions**
  - ? **1200 rpm, steady-state**
  - ? **6.7 bar IMEP load**
  - ? **Peak injection pressure = 1420 bar, 6 x 0.163 mm x 140° nozzle**
  - ? **Start of injection £ 4° BTDC**
  - ? **Start of combustion between 0° (TDC) and +0.5° ATDC**
  - ? **Simulated intake conditions: 53° C, 1.8 bar (abs.)**
  - ? **960 K, 31 kg/m^3 @ TDC (motored)**
  - ? **EGR simulated using nitrogen dilution**

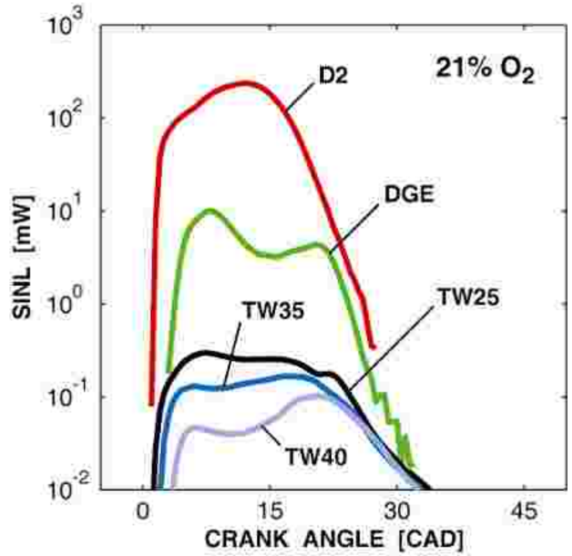
To What Extent Is DCDC Possible with Conventional and Emerging Fuels? [1,2]

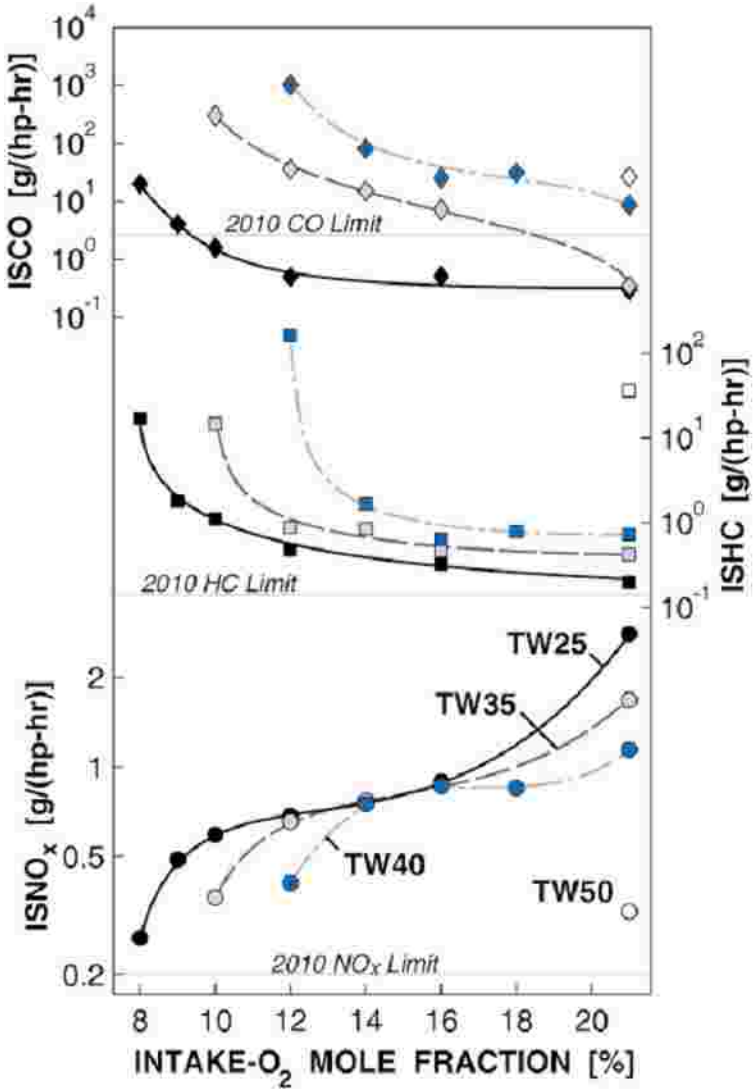
- **Answer: With near-term fuels, smoke emissions become ~50X too large at required EGR levels**
  - **Efficiency drops before compliant smoke emissions obtained**
  - **Highly oxygenated fuel can remove this barrier**
- **Very high levels of cooled EGR required for NO_x compliance**
  - **Is there a better way to introduce diluent?**



Are Fuel-Water Mixtures a Viable Alternative to EGR for NO_x Control? [3]

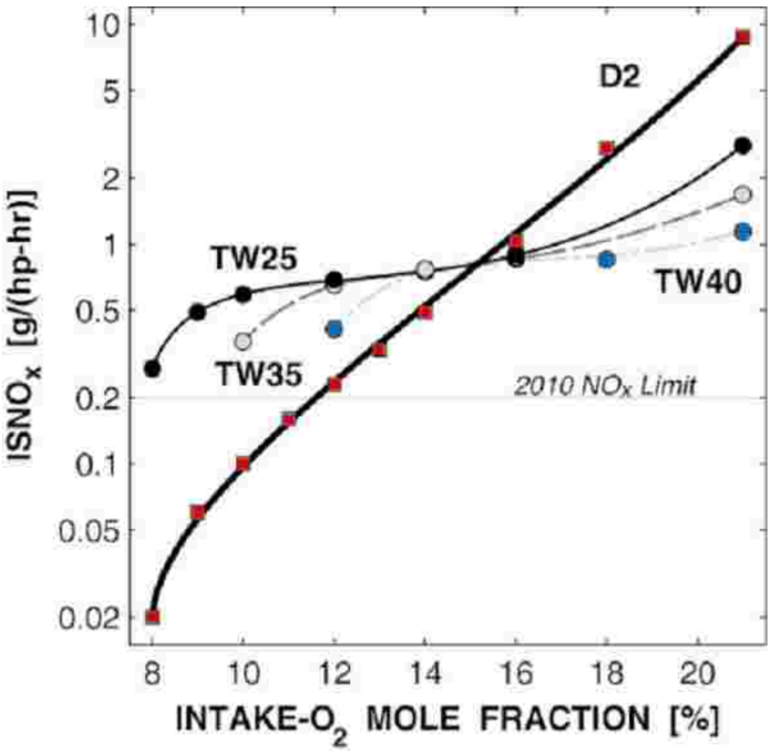
- **Answer: Yes, potentially**
  - ? Studied blends of tri-propylene glycol methyl ether with 25 to 50 vol% water
  - ? Stable blends pass corrosivity tests for ferrous metals and copper
  - ? Ignition delay » 40-50 cetane #2 diesel
  - ? Can lower NO_x by ~10x without using EGR (relative to #2 diesel)
  - ? HC and CO compliance possible with oxidation catalyst
  - ? Exceedingly low in-cyl. soot and engine-out smoke

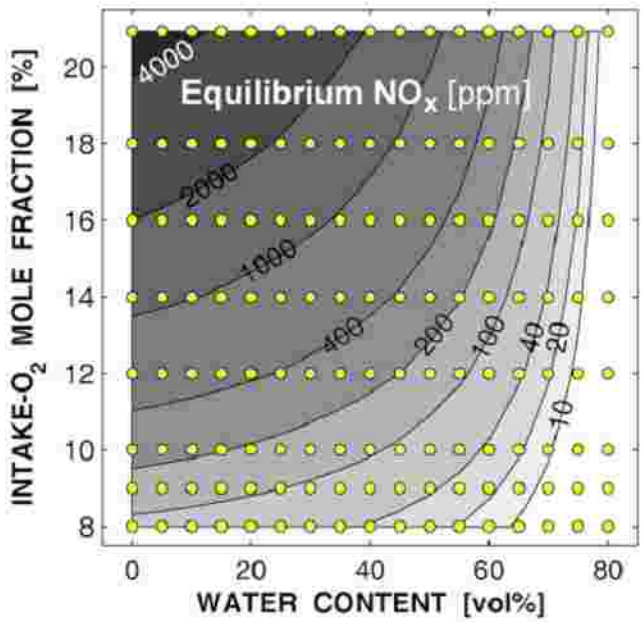




Are There Limitations to the Benefits of Fuel-Water Mixtures? [3]

- **Answer: Yes.**
  - ? **Incomplete combustion when > 40 vol% water**
  - ? **Even 10x lower NO_x isn't enough for 2010 compliance → need EGR or NO_x aftertreatment**
  - ? **NO_x doesn't decrease as rapidly as expected with simulated EGR**





- ? **Equilibrium calc's corroborate that NO_x doesn't decrease quickly with EGR @ high water content**
- ? **Even so, fuel-water mixtures could be part of a successful strategy**

Biodiesel NO_x [4]

NO_x emissions increase by ~1% for every 10 vol% biodiesel blended into diesel fuel.

Why?

Possible Reasons for Biodiesel NO_x Increase

- **Increased residence time at higher in-cylinder temperatures → higher NO_x**
  1. **Higher bulk modulus → earlier injection → earlier combustion**
  2. **Shorter ignition delay → earlier combustion**
  3. **Larger premixed-burn heat release**
  4. **Higher adiabatic flame temperature**
  5. **Less in-cylinder soot → less radiative heat transfer → higher actual flame temperatures**
  6. **Mixture-stoichiometry effects (thermal, chemical-kinetic)**
  7. **Others…?**

Experiment Design

- **Assess mechanisms 1-4 by comparing biodiesel results to those using a hydrocarbon reference fuel with same:**
  1. **Injection timing to remove bulk-modulus effect**
  2. **Start of combustion to remove combustion-phasing effect**
  3. **Ignition delay to remove premixed-burn magnitude effect**
  4. **Adiabatic flame temperature**

If above matching is accomplished

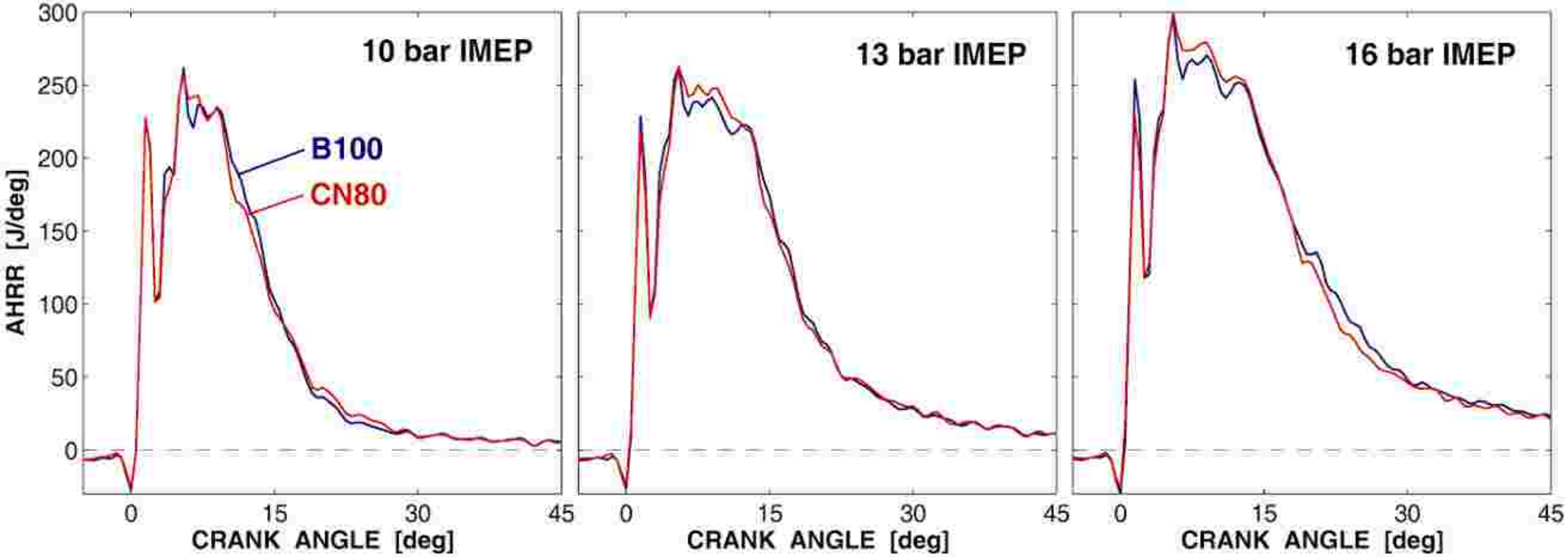
and differences in one (or more) of these is primary cause of biodiesel NO_x increase

then biodiesel NO_x increase should vanish.

Fuels and Operating Conditions

- **Fuels**
  - ? **B100 = neat soy biodiesel (Peter Cremer Nexsol BD-0100)**
  - ? **CN50 = 50-cetane blend of diesel primary reference fuels (PRFs), 41.2 vol% *n*-hexadecane + balance 2,2,4,4,6,8,8-heptamethylnonane**
  - ? **CN80 = 80-cetane PRF blend, 76.5 vol% *n*-hexadecane + balance heptamethylnonane**
  - ? **CN100 = 100-cetane PRF (*i.e.*, neat *n*-hexadecane)**
- **Operating conditions**
  - ? **Selected to maximize NO_x differences between B100 and PRFs**
  - ? **800 rpm, steady-state, 0% EGR, conventional injection timing, start of combustion between 0° (TDC) and +0.5° ATDC**
  - ? **Loads from 10 to 16 bar gross IMEP in 1-bar increments**
  - ? **Peak injection pressure = 1420 bar, 6 x 0.163 mm x 140° nozzle**
  - ? **Simulated intake conditions 69°C, 1.43 bar for 16:1 CR engine**
  - ? ^{3} **4 repeats at each operating condition**

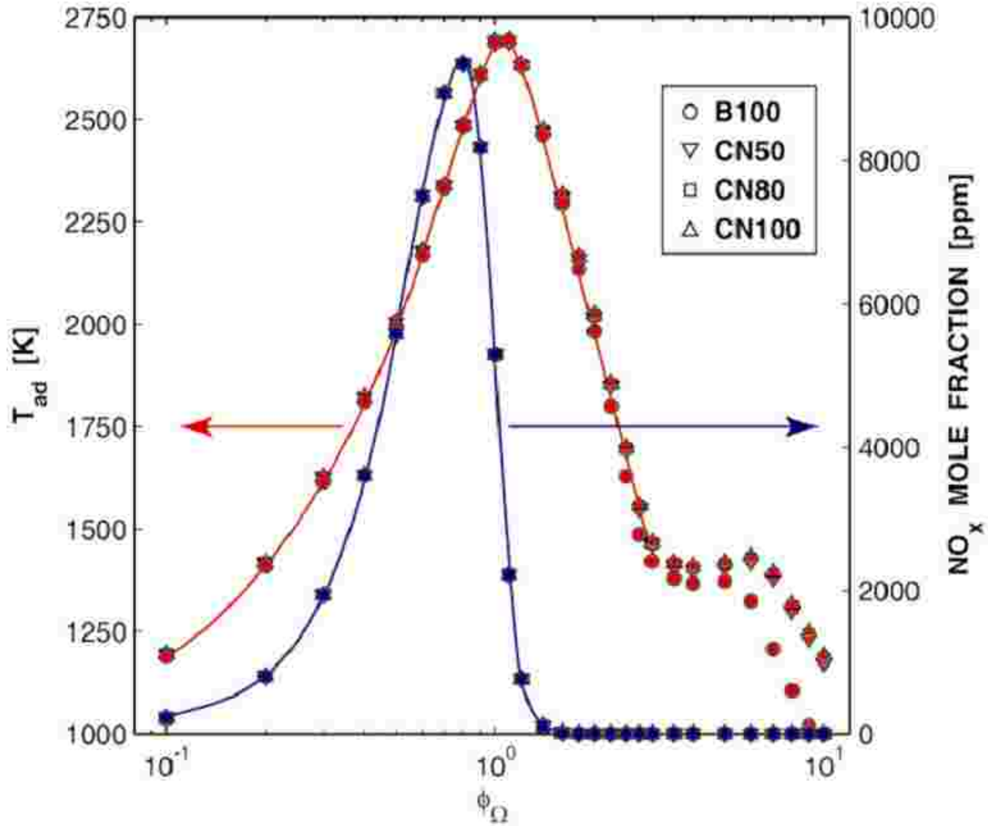
Similar AHRR Curves for B100 and CN80



- **Start of injection, start of combustion, and premixed-burn magnitude well matched across load range**
- **Mixing-controlled heat release also well matched**
  - ? **15% lower LHV of B100 is mostly offset by 12% higher density → injection duration approx. same as for CN80**

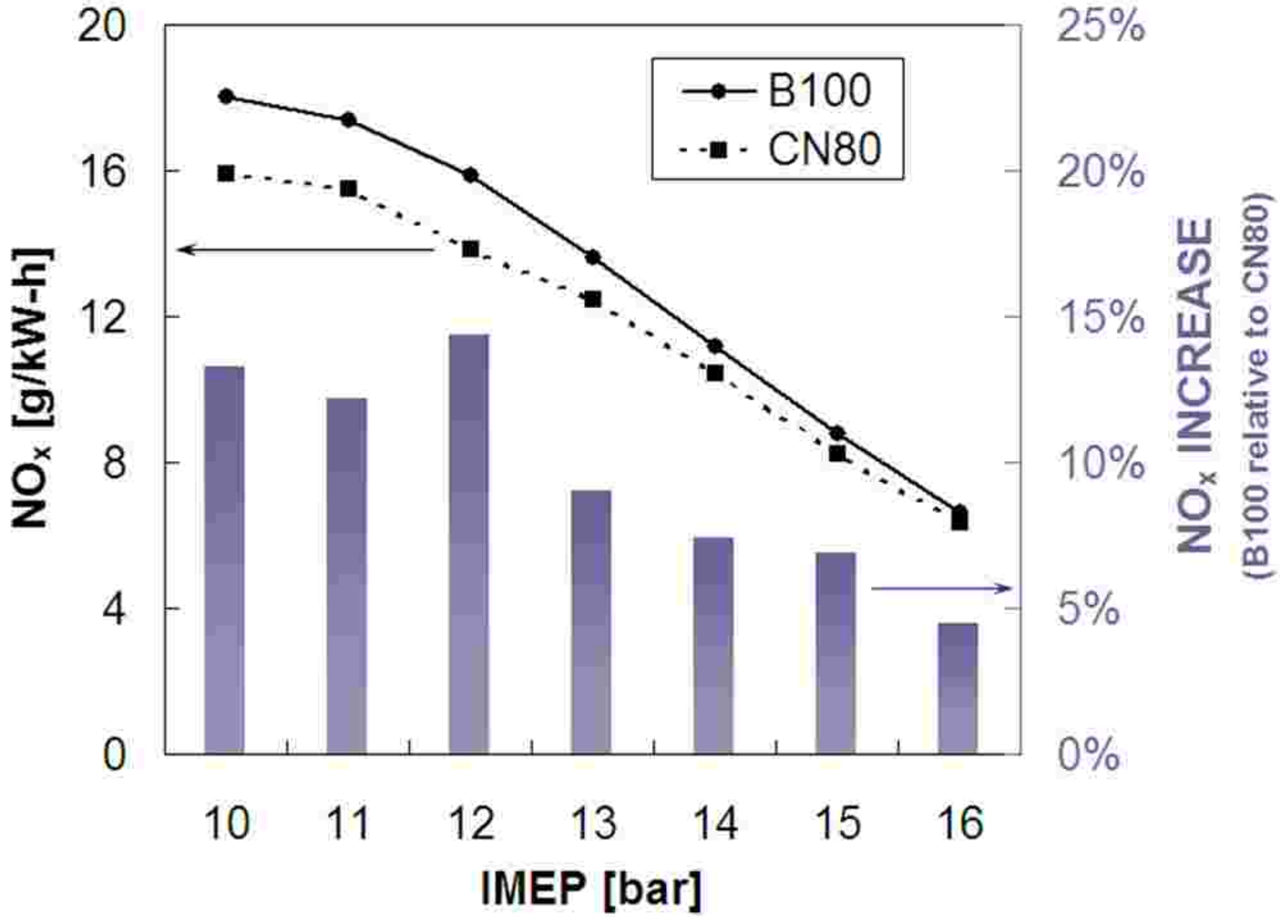
Adiabatic Flame Temperature (T_{ad}) Effects

- **Methyl oleate (C18:1) used as surrogate for B100**
- **EQUIL module of CHEMKIN software used to compute T_{ad}**
  - ? **Initial conditions: 950 K, 23 kg/m³**
- **No differences in T_{ad} observed at $f_w = 1.0$**
  - ? **B100 LHV is lower but $(F/O)_{st}$ is larger → effects exactly compensate for one another**



T_{ad} differences do not appear to be cause of increased biodiesel NO_x

NO_x Is 10.5% Higher for B100 Than CN80



Factors other than ignition delay, start of combustion d premixed-burn magnitude contribute to increased biodiesel NO_x

Conclusions

- **Dramatic fuel changes can enable mixing-controlled HECC, avoiding common problems of more-premixed LTC strategies**
  - ? **No problems with ignition-timing control, light-load misfire, or high-load knock and NO_x**
- **Nevertheless, significant technical advancements are required to enable *practical* mixing-controlled HECC**
  - ? **Mixture preparation and fuel must be optimized togethe to avoid:**
    - † Excessive EGR requirements for NO_x control
    - † High smoke emissions with current and emerging fuels
- **Current hypotheses are inadequate to explain the NO_x increase when fueling with biodiesel (relative to a diesel PRF blend)**
  - ? **Changes in start of injection, start of combustion, premixed-burn magnitude, and adiabatic flame temperature are not con rolling factors over a range of load conditions**
  - ? **Differences in radiant heat transfer and/or mixture stoichiometry could play roles (investigation underway)**

Acknowledgments

Dr. Glen C. Martin – ***post-doc***

Caterpillar Inc. – ***hdwe. support, guidance***

Dr. Ansis Upatnieks – ***former post-doc***

Prof. A.S. (Ed) Cheng – ***collaborator***

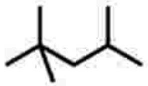
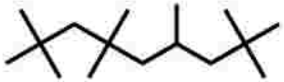
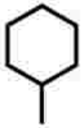
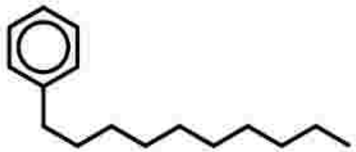
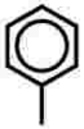
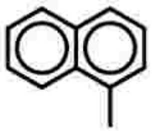
Dr. Randy L. Vander Wal – ***collaborator***

Advanced Engine Combustion,
Diesel Surrogates – ***working groups***

Questions

What Compounds Should Be Used to Create a Diesel Surrogate for Kinetics Studies? [5]

- **Answer: Diesel Surrogates Working Group has selected…**

Near-Term		Longer-Term	
n-decane ($C_{10}H_{22}$)		*n*-hexadecane ($C_{16}H_{34}$)	
iso-octane (C_8H_{18})		heptamethylnonane ($C_{16}H_{34}$)	
methyl cyclohexane (C_7H_{14})		*n*-decylbenzene ($C_{16}H_{26}$)	
toluene (C_7H_8)		1-methylnaphthalene ($C_{11}H_{10}$)	

? **Compounds can be blended to match characteristics of r diesel: ignition delay, molecular structures, C/H ratio, volat ity, …**

? **Compounds readily obtainable for experimental research forts**

? **Detailed kinetic mechanisms already exist or can be developed**

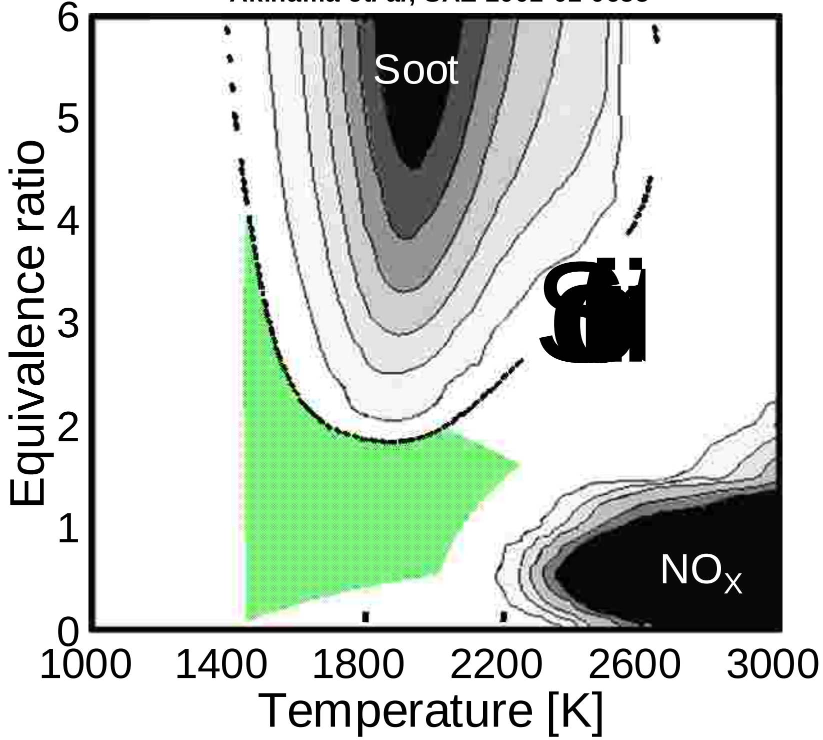
How to Quantify Mixture Stoichiometry Once Reactions Have Begun? [6]

- **Answer: The oxygen equivalence ratio, f_{w}**

$$f_{\Omega} \equiv \frac{2n_C + \frac{1}{2}n_H}{n_O}$$ **, neglecting atoms bound in CO_2 and H_2O**

- **Important for tracking reaction progress in (f,T) space**
- **Important when oxygenated fuels are used (*e.g*., biodiesel, ethanol, DME, …)**
- **Same as traditional f definition before reactions have begun**
  - ? **As long as fuel not oxygenated**
  - ? **General relationship between f and f_{w} provided**

Akihama *et. al*, SAE 2001-01-0655



How to Quantify Degree of Achievement of Many Simultaneous Operational Targets? [2]

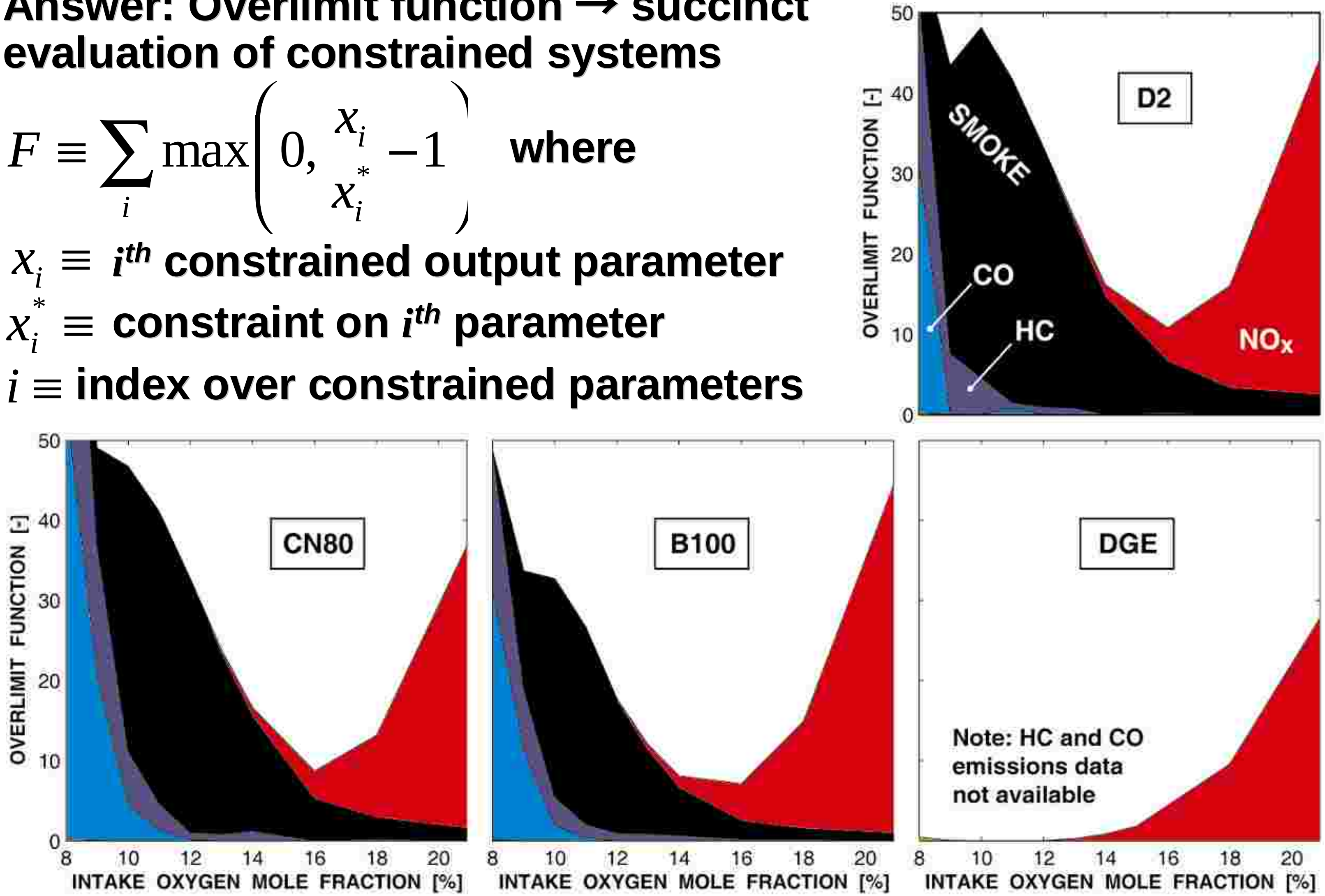
- **Answer: Overlimit function → succinct evaluation of constrained systems**

$$F \equiv \sum_i \max\left(0, \frac{x_i}{x_i^*} - 1\right)$$ **where**

$x_i \equiv$ ***i^th^*** **constrained output parameter**

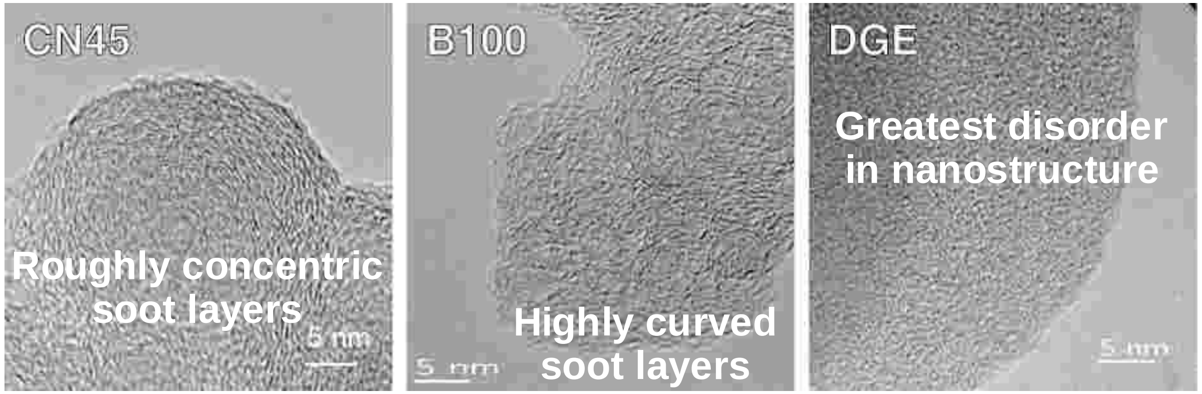
$x_i^* \equiv$ **constraint on** ***i^th^*** **parameter**

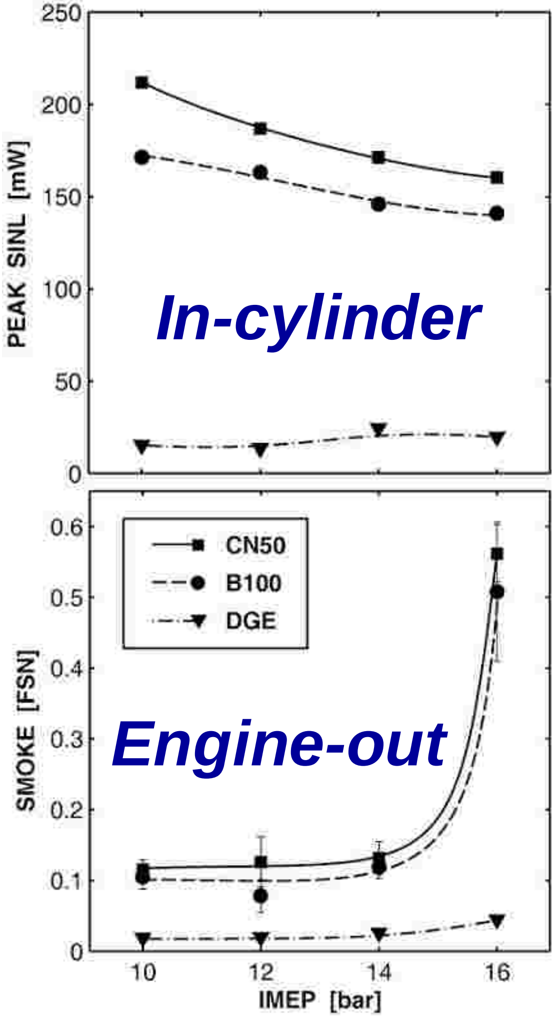
$i \equiv$ **index over constrained parameters**



Could Fuel Effects on Soot Nanostructure Affect Emissions? [7]

- **Answer: Yes.**
  - ? **Soot with less-ordered nanostructure oxidizes up to 5X faster**
  - ? **Soot produced by different fuels has different nanostructure (similar operating conditions)**
    - † Hydrocarbon ref. fuel → highly ordered soot
    - † Neat biodiesel → less order in nanostructure
    - † DGE → greatest disorder in nanostructure
  - ? **DGE soot has shortest fringe lengths and largest tortuosity → enhanced oxidation rate**





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