An Experimental Investigation of the Origin of Increased NOx Emissions When Fueling a Heavy-Duty Compression-Ignition Engine with Soy Biodiesel

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Motivation

- NO_x increase is barrier to full biodiesel market penetration in US
  - California and Texas prohibit NO_x-increasing fuels/additives
- Previous work has shown NO_x increase can originate from
  - Combustion effects
  - Engine-calibration effects (see SAE 2008-01-0078)
- Combustion effects not well understood (many hypotheses)

Identification of underlying cause(s) of biodiesel NO_x increase is a key step in developing successful mitigation strategies

Objective

Understand combustion mechanism(s) underlying the biodiesel NO_x increase

- Determine magnitude of NO_x increase under conventional and emerging operating modes
- Evaluate validity of primary hypotheses
- Give insights into origins of NO_x increase that are relevant for all fuels

Hypotheses for Biodiesel NO_x Increase

- Most hypotheses are based on increased thermal-NO_x formation

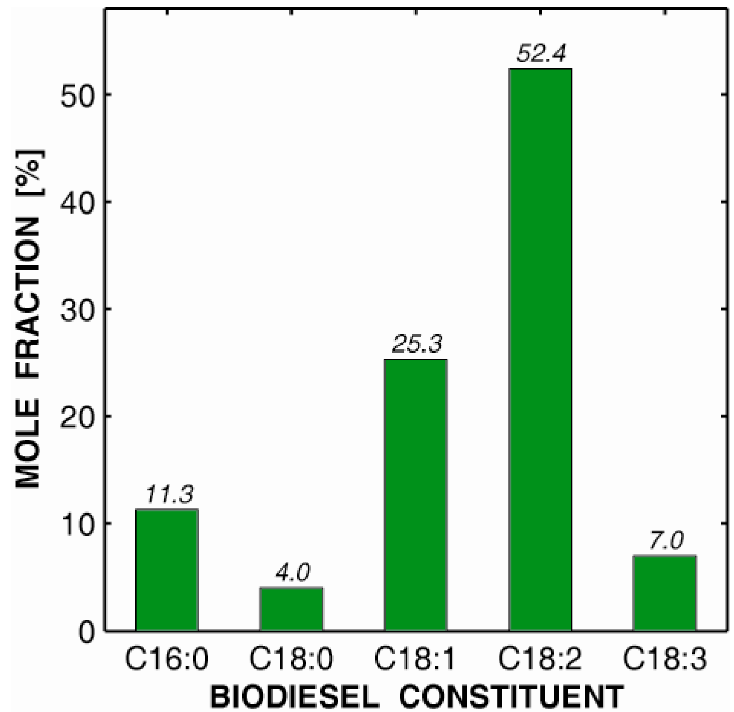
> ***Increased in-cylinder temperature and/or residence time at high temperature will increase thermal NO_x***

1. Increased fraction of premixed combustion
2. Increased peak bulk-gas-averaged temperature
3. Higher adiabatic flame temperature
4. Higher actual flame temperature ← lower radiative heat loss
5. Faster combustion
6. Autoigniting/reacting mixtures closer to stoichiometric

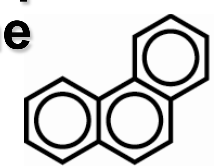
- Other hypotheses focus on increased prompt-NO_x formation
  - Not investigated in this work

Fuels

- **B100**: neat soy biodiesel (Peter Cremer Nexsol BD-0100)
  - Methyl palmitate (C16:0)
  - Methyl stearate (C18:0)
  - Methyl oleate (C18:1)
  - Methyl linoleate (C18:2)
  - Methyl linolenate (C18:3)

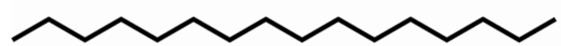


- **B94**: B100 doped with 6 wt% phenanthrene

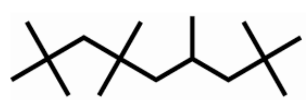


phenanthrene ($C_{14}H_{10}$)

- **CN45** and **CN70**: 45- and 70-cetane diesel primary reference fuel mixtures



n-hexadecane ($C_{16}H_{34}$)

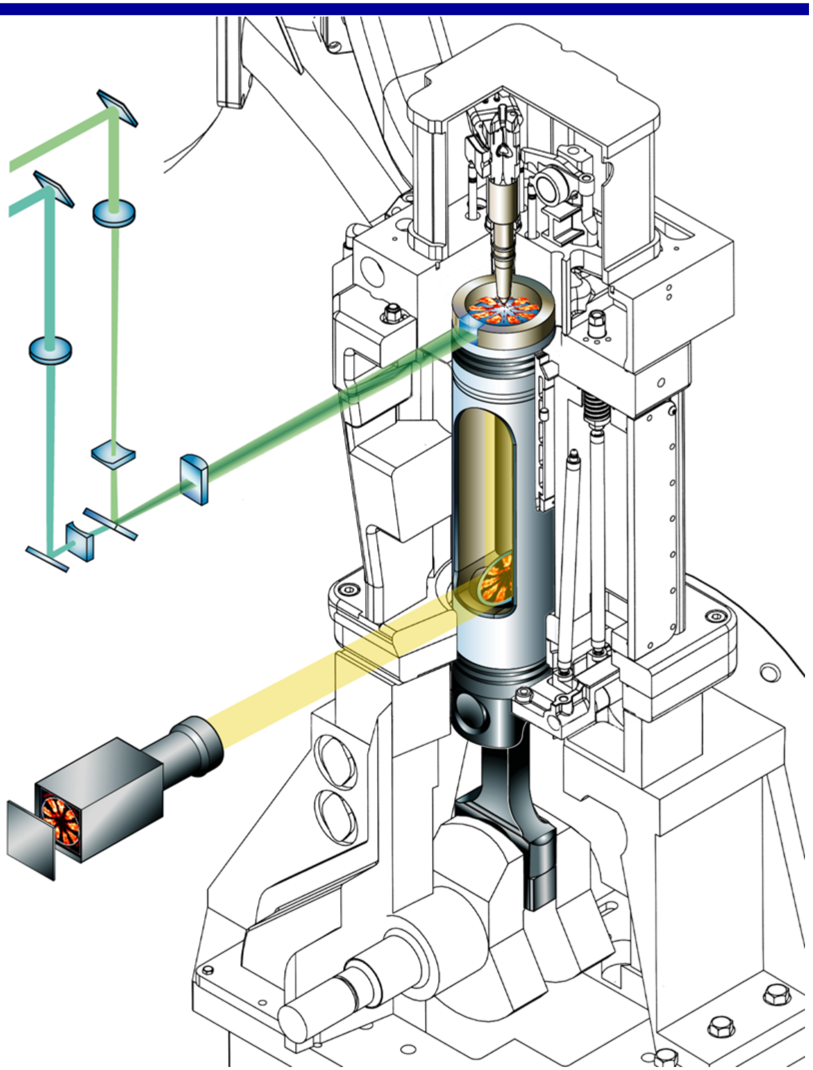


heptamethylnonane ($C_{16}H_{34}$)

- Ign. delay, start of combustion matched for **B100**, **B94**, and **CN45**

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
Displacement per cyl.	1.72 liters
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
Compression ratio	11.75:1
Simulated compr. ratio	16.00:1
Fuel injector type	Cat HEUI A
Fuel injector orifices	6 x .163 mm x 140°
Injection press. (nom.)	142 MPa



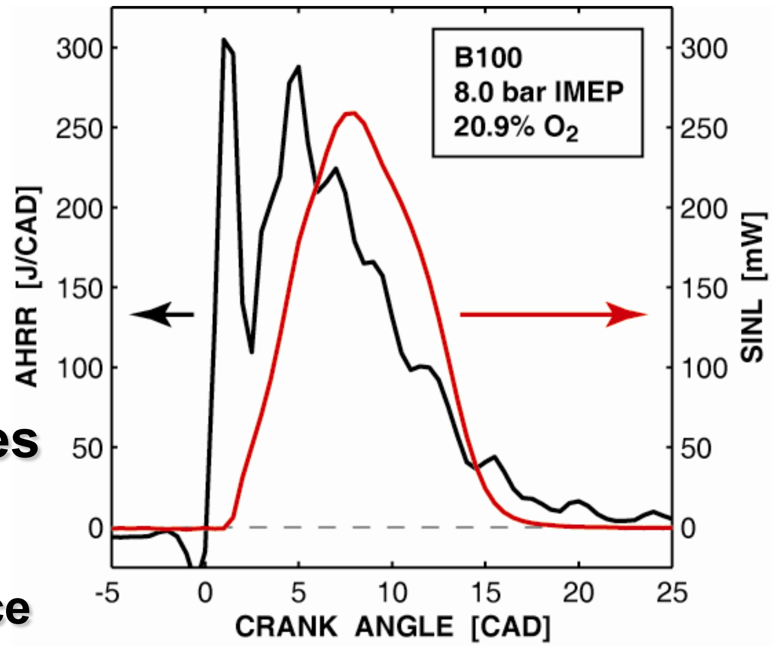
Operating Conditions

Engine speed	800 rpm (steady-state)	
Engine loads	4.0, 8.0, 12.0, 15.0 bar IMEP	
Start of injection	-2.2 to -1.0° ATDC	
Start of combustion	-0.1 to +0.5° ATDC	
Intake-O_2 mole fractions	20.9%	16.5%
Motored TDC temperature	910 K	850 K
Motored TDC pressure	63 bar	77 bar
Motored TDC density	24 kg/m^3	32 kg/m^3

- Simulated exhaust gas recirculation (EGR):
  - N_2 and CO_2 added to intake air to match O_2 mole fraction and specific heat at TDC of in-cylinder mixture with real EGR

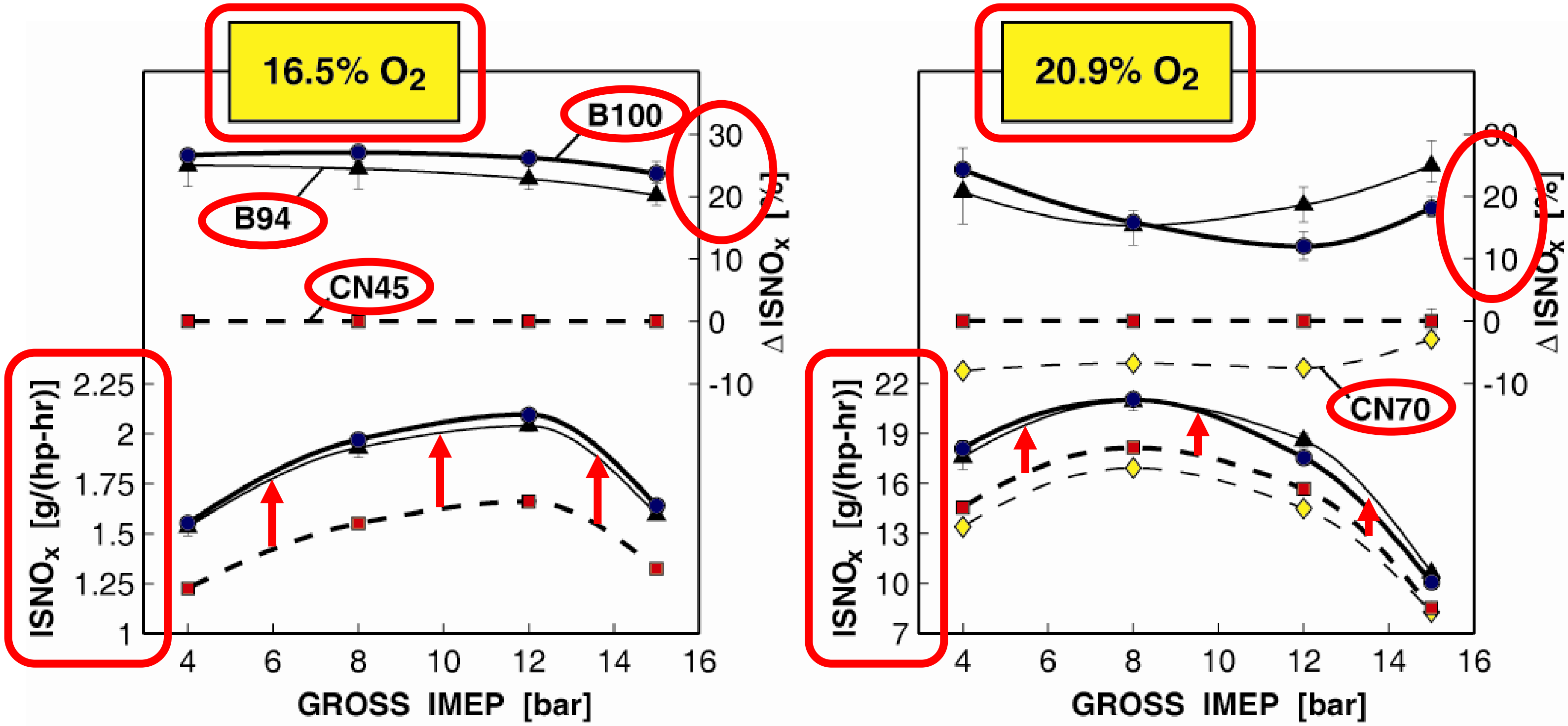
Diagnostics

- **Cylinder pressure →**
  - Apparent heat-release rate (AHRR)
  - Start of combustion
  - Combustion phasing



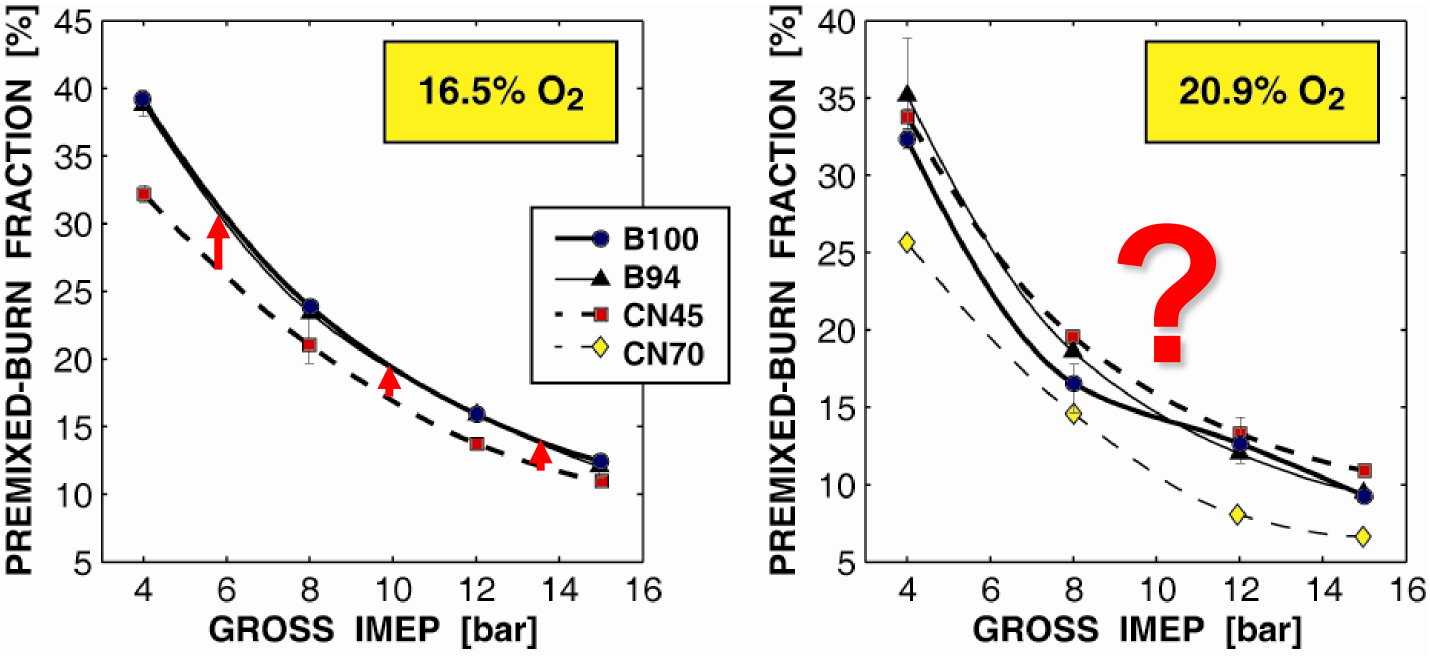
- **Spatially integrated natural luminosity (SINL) →** measure of radiative heat loss from in-cylinder gases
- **Engine-out emissions**
  - NO_x using heated chemiluminescence detector (CAI Model 600 HCLD)
  - Smoke using smokemeter (AVL Model 415S)
- **Chemiluminescence imaging (310 nm) →** flame lift-off length
- **Mie-scattered light imaging (532 nm) →** actual start of injection
- **Average mass of fuel per injection →** indicated efficiency

Results: EGR and Load Effects on NO_x Emissions



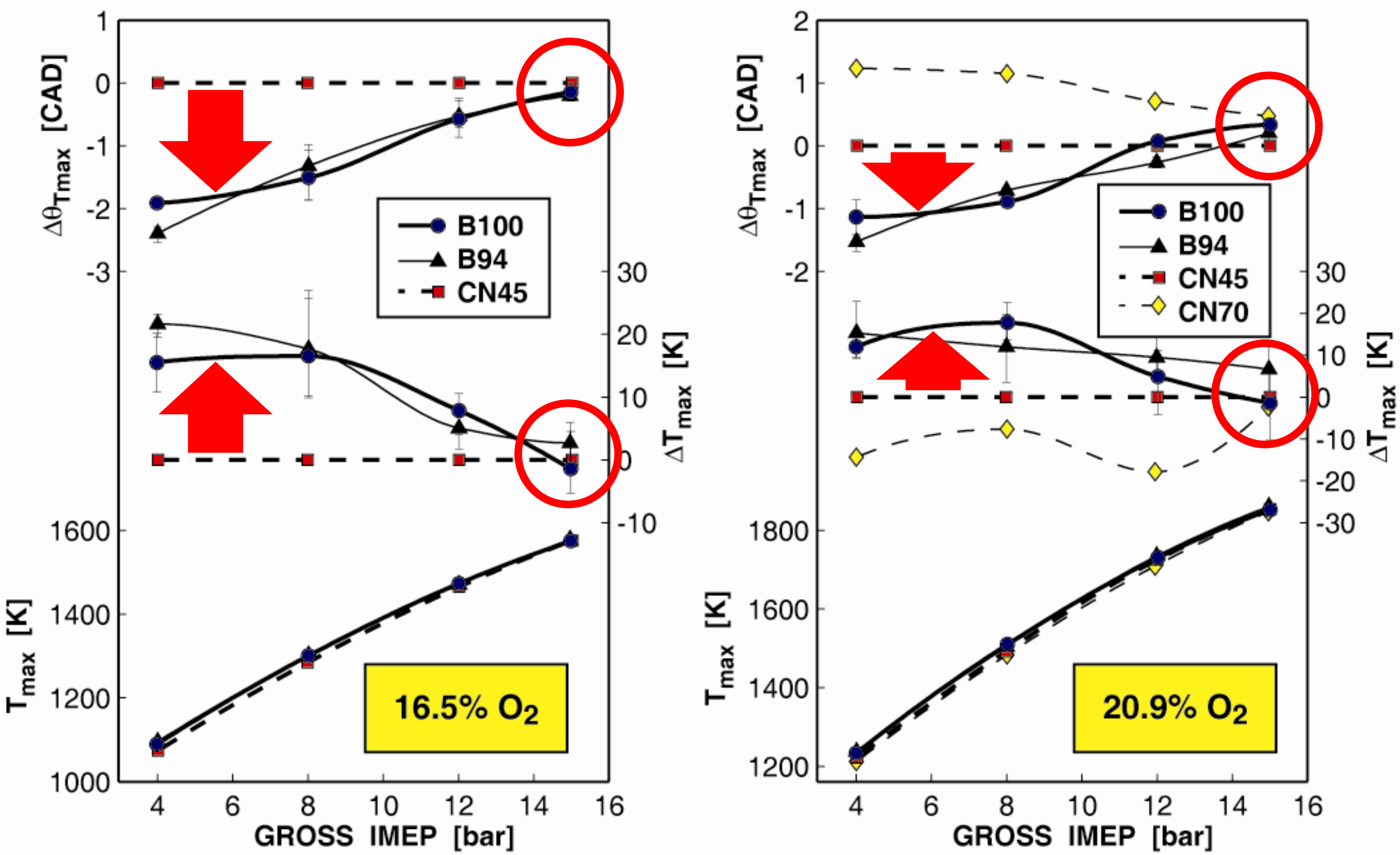
- EGR lowers $ISNO_x$, biodiesel fuels (BDFs) exhibit highest $ISNO_x$
- Load-averaged B100 $ISNO_x$ increase is larger with EGR addition
  - 26% $ISNO_x$↑ with moderate EGR *vs*. 18% $ISNO_x$↑ without EGR

Premixed-Burn Fraction Cannot Explain Biodiesel NO_x↑ at 20.9%-O_2 Condition



- Solid lines = BDFs, dashed lines = hydrocarbon fuels
- BDFs have consistently larger premixed-burn fractions at 16.5% O_2, but correlation breaks down at 20.9% O_2

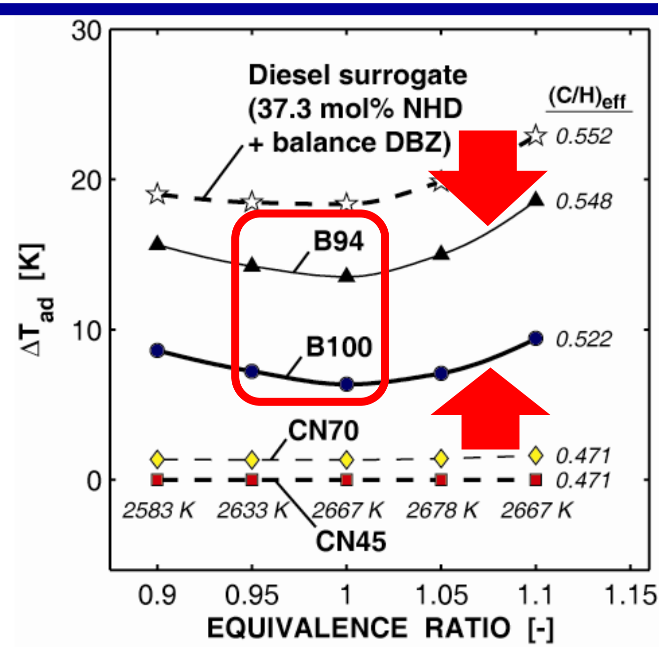
Peak Bulk-Gas-Averaged Temperature (T_{max}) Cannot Explain Biodiesel NO_x↑ at High Load

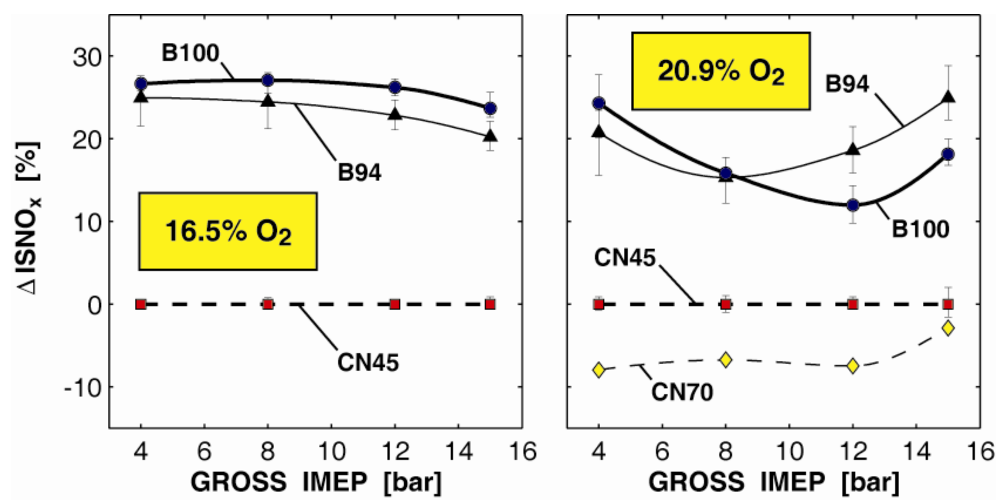


- T_{max} generally is larger and occurs earlier for BDFs
- T_{max} differences disappear at highest loads

Fuel Effects on Adiabatic Flame Temp. (T_{ad}) Cannot Fully Explain Biodiesel NO_x↑

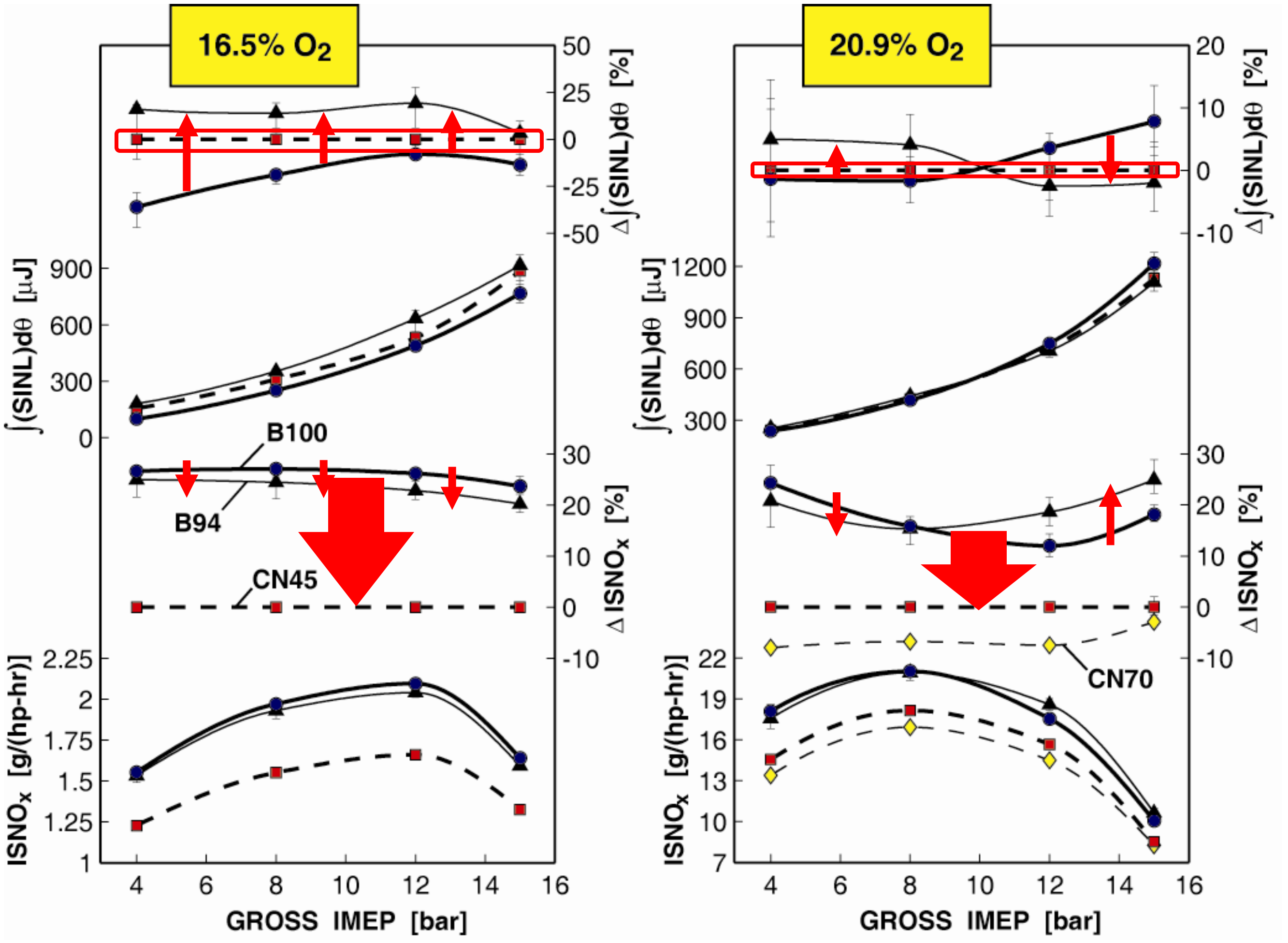
- T_{ad} values are:
  - Lower for BDFs than for diesel-like fuel
  - Higher for BDFs than for CNxx
- If T_{ad} differences were the controlling factor for NO_x, then
  - BDFs would have lower NO_x than conventional diesel
  - B94 would always have significantly higher NO_x than B100
  - CN70 would have higher NO_x than CN45





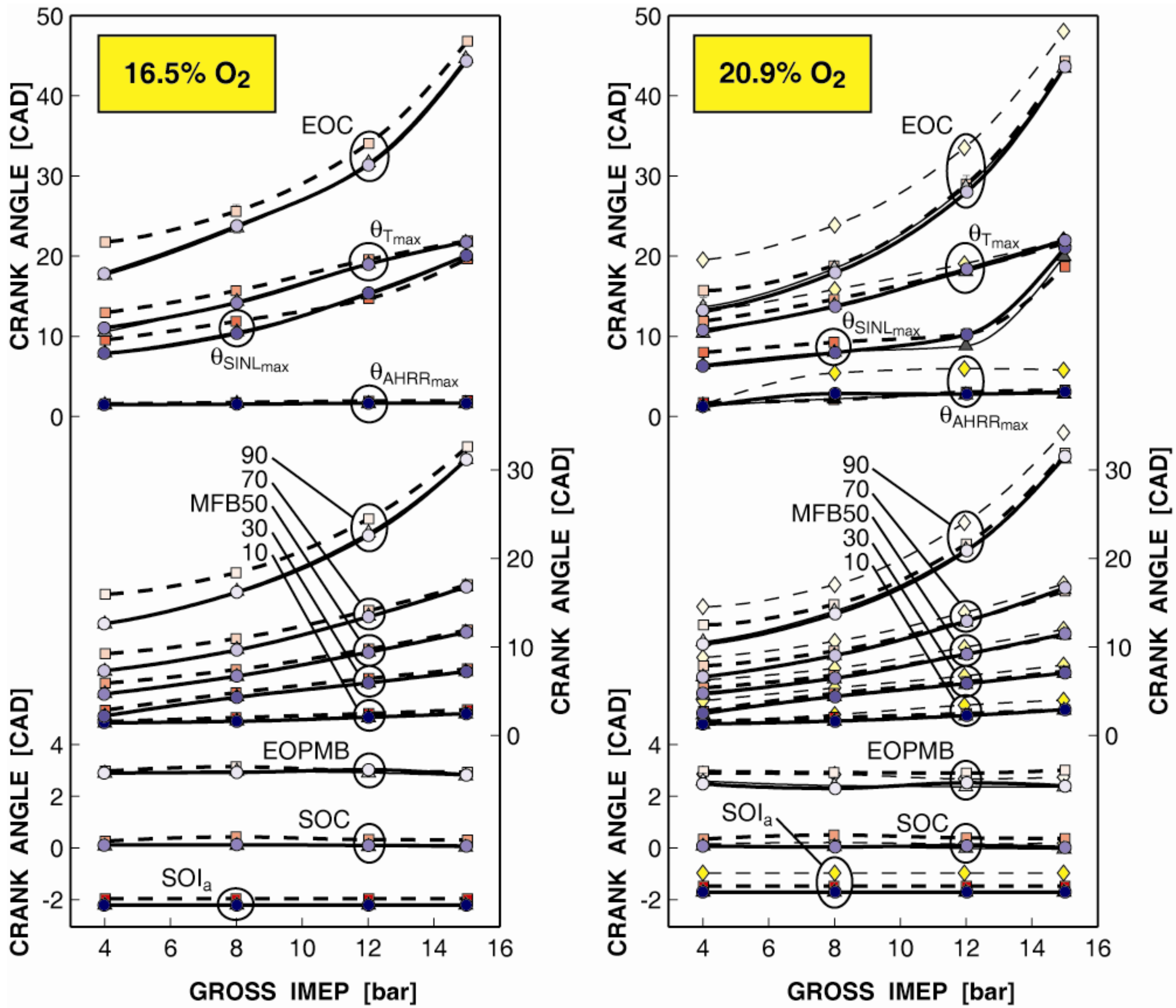
Radiative Heat Transfer Likely Important, but Cannot Fully Explain Biodiesel NO_x↑

- Changes in integrated SINL correlate with NO_x changes for B100 and B94
- CN45 doesn't show same trend



Combustion Phasing Effects Are Correlated with Biodiesel $NO_x\uparrow$

- Solid lines = BDFs, dashed lines = hydrocarbon fuels
- Combustion occurs more quickly for BDFs
  - Even though injection durations are longer at constant load



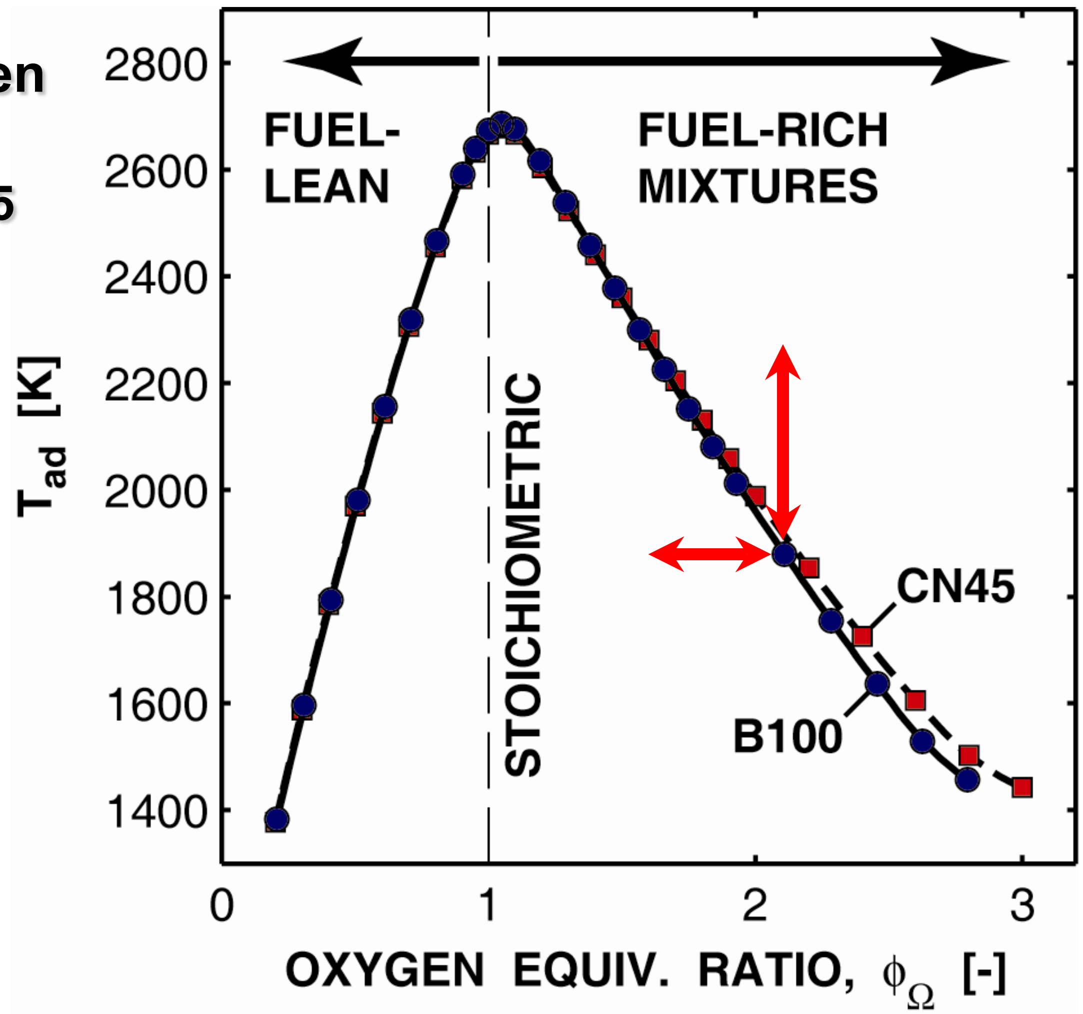
Summary of Understanding to This Point

- NO_x increase for B100 relative to CN45 is 18% without EGR, 26% at moderate-EGR conditions
- None of the following effects are perfectly correlated with observed NO_x changes (but any/all could play roles)
  - Premixed-burn fraction
  - Peak bulk-gas-averaged in-cylinder temperature
  - Adiabatic flame temperature
  - Radiative heat transfer
- B100 and B94 exhibit faster combustion
  - Longer residence time at high temperature → higher NO_x
  - What causes the faster combustion?
- Still don't really understand origin of the biodiesel NO_x increase!
  - What about mixture-stoichiometry effects?

Mixtures That Are Closer to Stoichiometric Yield Higher Product Temperatures

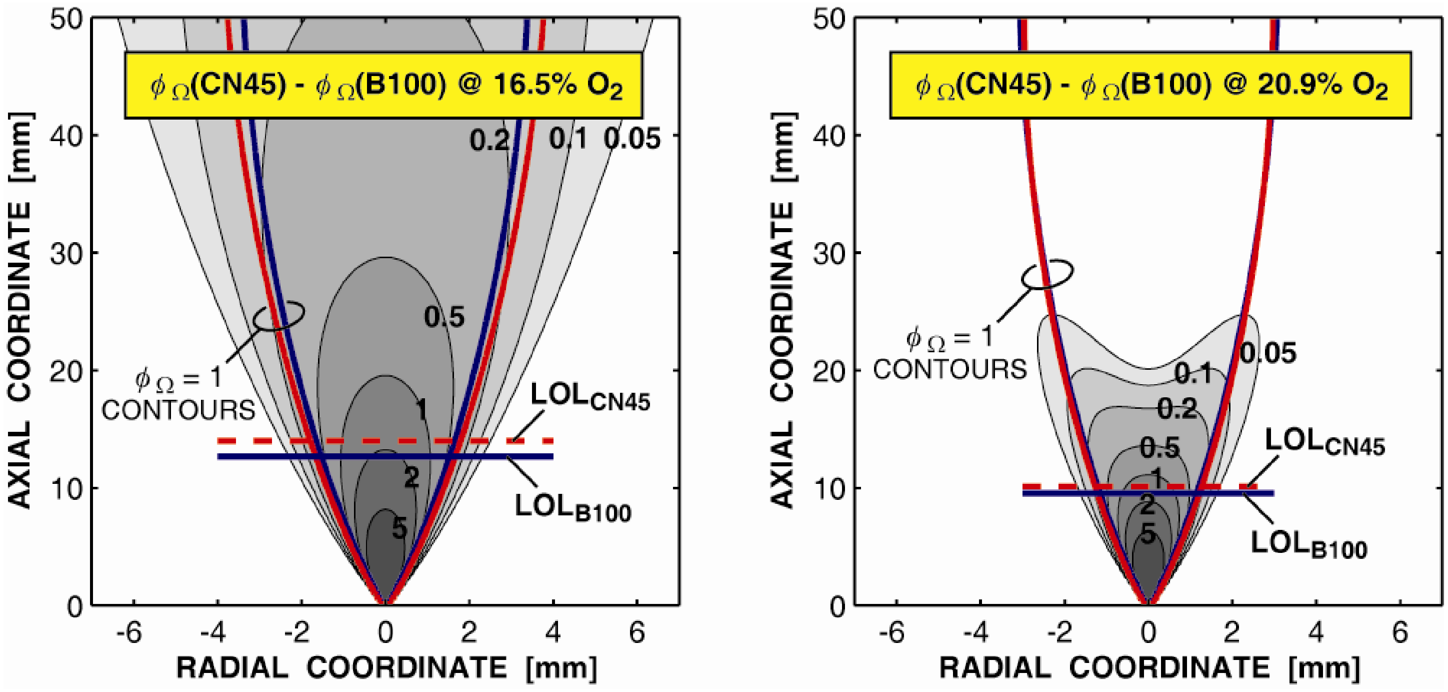
- **Mixture stoichiometry quantified using oxygen equivalence ratio, ϕ_Ω**
  - **See SAE 2005-01-3705**

- **Relatively small ϕ_Ω changes (~0.5) can lead to large differences (100-400 K) in product-mixture temperature**



Biodiesel Mixtures Are Closer to Stoichiometric over Broad Regions

- ϕ_Ω fields estimated using mixing model (SAE 1999-01-0528) and validated radial mixture distribution (*IJER* **7**:103, 2006)

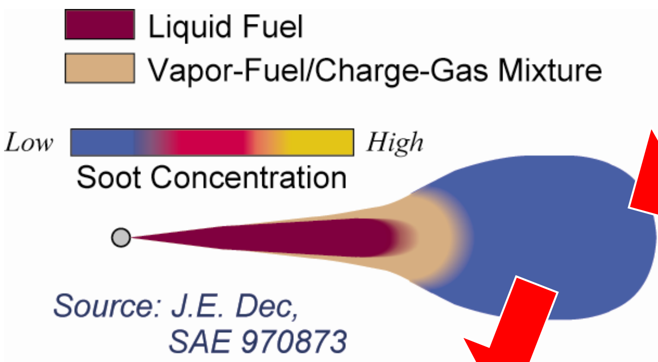


- ϕ_Ω closer to stoichiometric for B100 (and B94) than for CN45
  - Throughout jet at ignition and at the lift-off length (LOL)

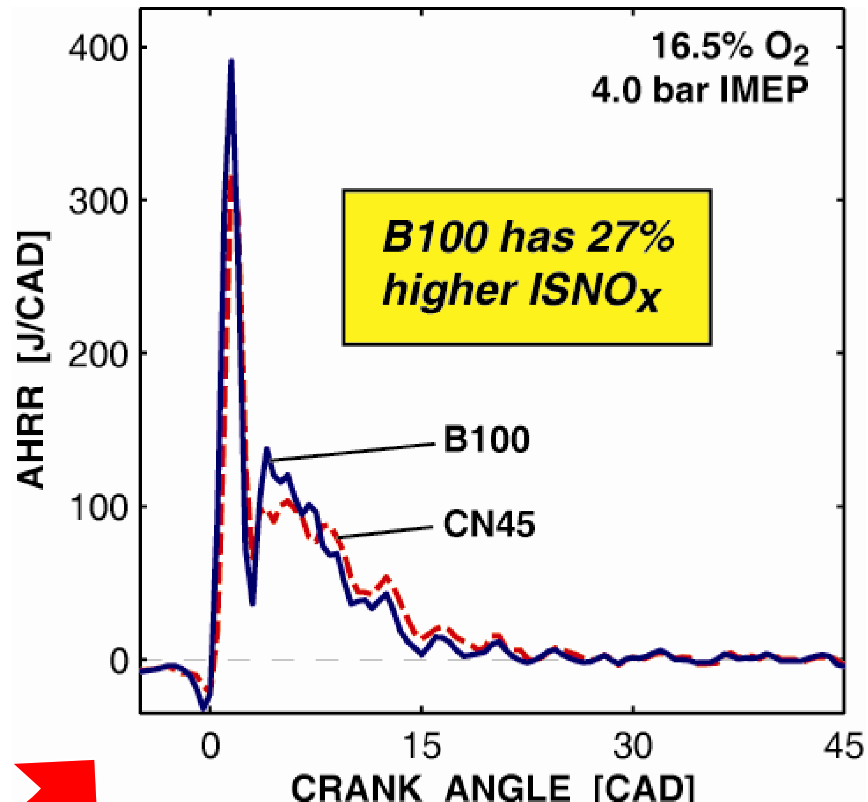
Conclusions

Under Premixed-Ignition Conditions, the Biodiesel NO_x Increase is Caused by…

- **Reacting mixtures closer to stoichiometric during ignition**

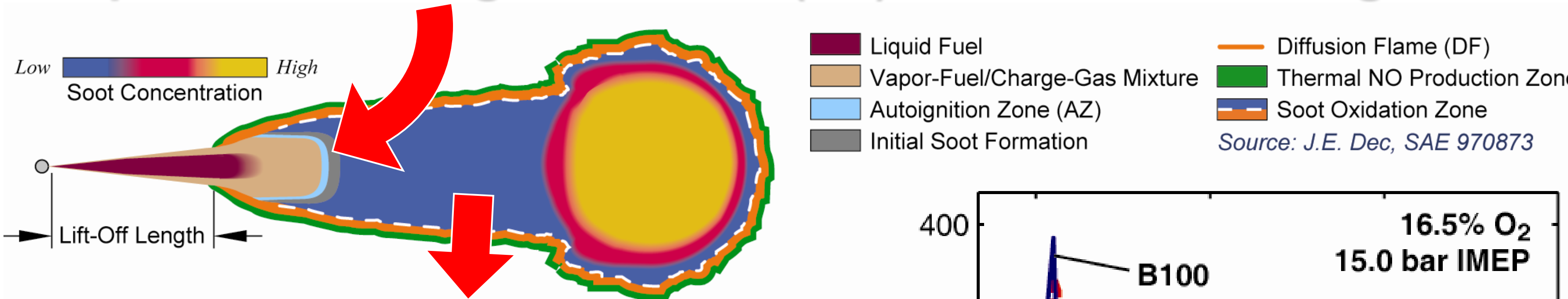


- **Higher temperatures**
  - Faster reaction rates
- **Less mixing-controlled combustion required for complete oxidation**
- **Shorter combustion duration**
- **Longer residence time at higher temperature**
- **More thermal NO_x**

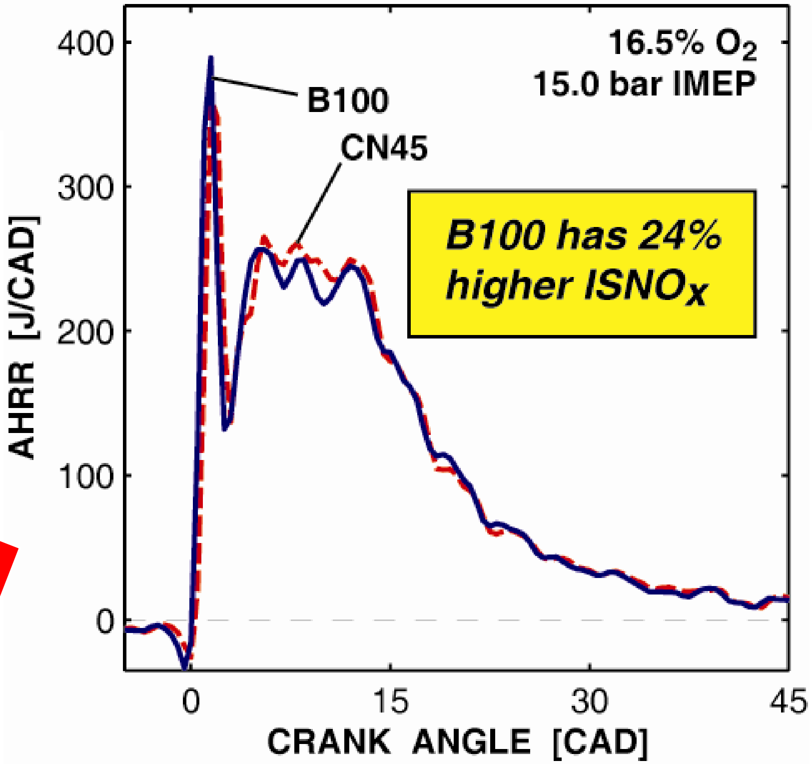


Under Higher-Load Conditions the Biodiesel NO_x Increase is Caused by…

- **Reacting mixtures closer to stoichiometric in the standing premixed autoignition zone (AZ) near the lift-off length**



- **Same premixed-ignition phenomena**
  - Higher temperatures, less mixing-controlled combustion required
- **Also less soot → less radiative heat loss → higher local temperatures**
- **More thermal NO_x**



Final Notes

- Primary factor in biodiesel NO_x increase appears to be igniting/ reacting mixtures that are closer to stoichiometric
  - Consequences are: larger premixed burn, higher temperatures, faster combustion, less radiative heat loss → more thermal NO_x

See SAE 2009-01-1792 for details

- Preceding conceptual understanding is consistent with trends observed in current work and in literature, but remains to be rigorously validated
- Optimizing an engine for biodiesel use is likely to provide benefits relative to an engine optimized for diesel
  - Some fraction of biodiesel PM, HC, and CO benefits can be traded off to eliminate NO_x increase (*e.g.*, by adding EGR) and raise efficiency (*e.g.*, by decreasing DPF regeneration frequency)

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