Fuel Flexibility and Reactivity Controlled Compression Ignition (RCCI)

Rolf D. Reitz

Engine Research Center, University of Wisconsin-Madison

Workshop on Techniques for High-Pressure Combustion
August 29 - September 1, 2011
Argonne National Laboratory, Argonne, Illinois 60439 USA

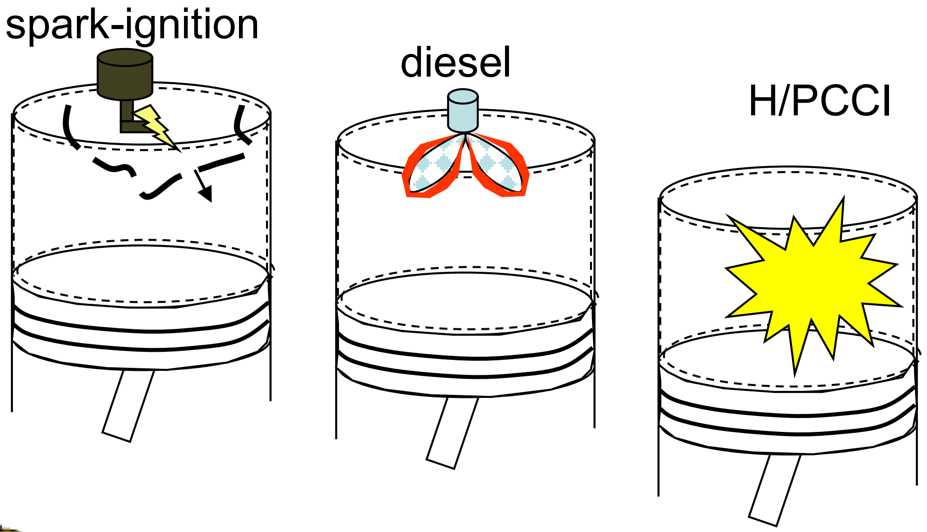
Acknowledgments
DERC Member Companies, DOE/Sandia National Labs
Oak Ridge National Labs, ERC Students and Staff

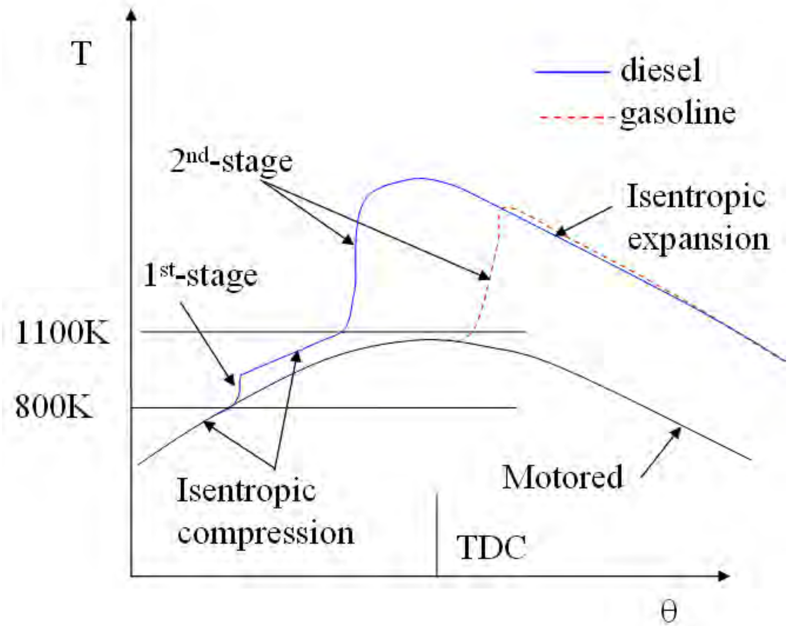
Outline

- RCCI combustion background
- Experimental engines
- Modeling and experimental results
- Use of renewable fuels – hydrated ethanol/diesel
- Optimization of combustion chamber geometry
- RCCI combustion mechanisms and soot modeling
- Conclusions and future research directions

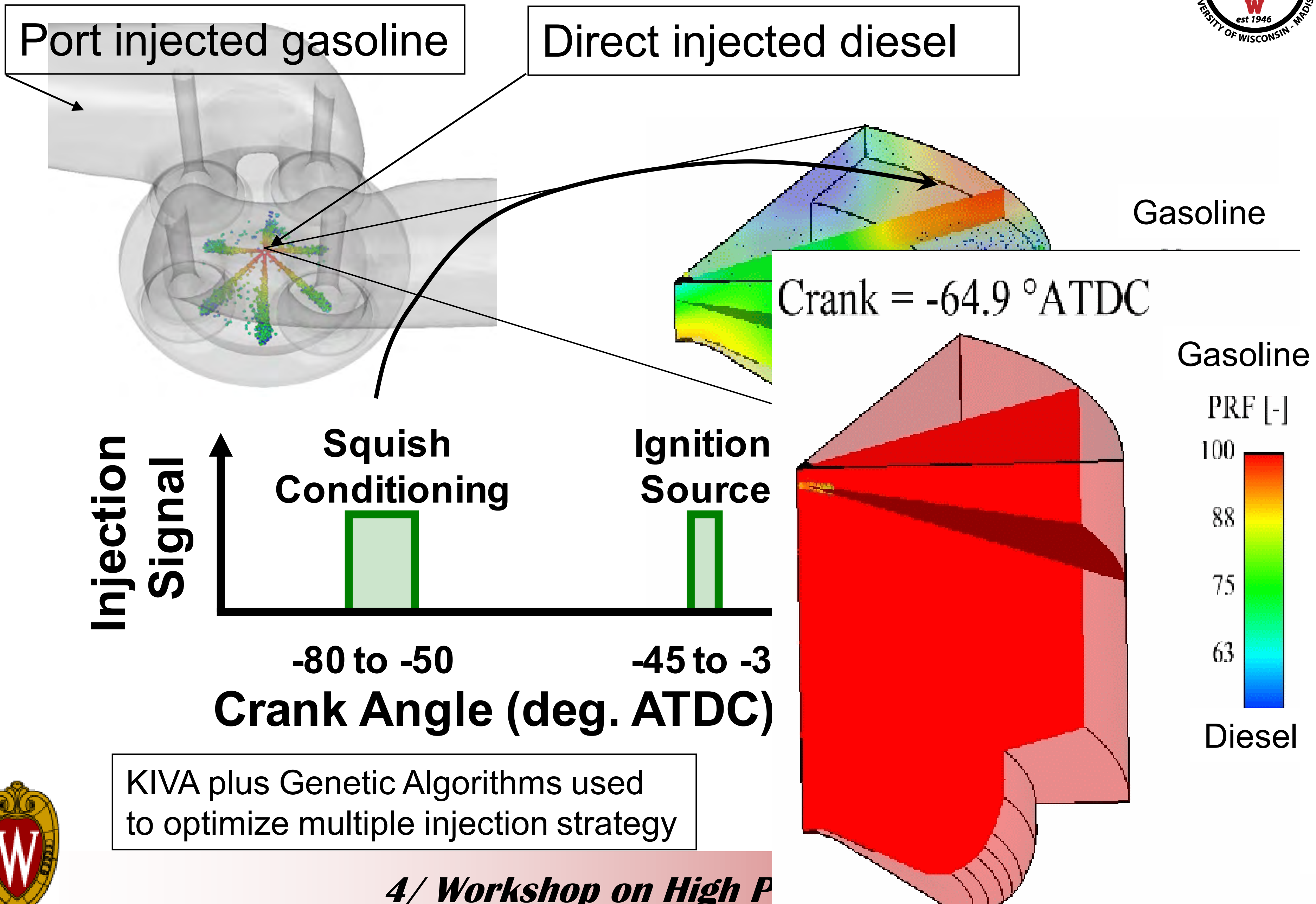
IC engine combustion regimes

- Gasoline engine spark-ignition with flame propagation:
  High turbulence for high flame speed → heat losses, NOx and UHC/CO
  knock (CR, fuels), throttling losses → low thermal efficiency TE ~25%
- Diesel engine with spray (diffusion) combustion:
  Rich mixtures (soot), high temperatures (NOx) → higher TE ~45%
- H/Premixed Charge Compression Ignition – LTC, chemistry controlled:
  Sensitive to fuel, poor combustion/load control, low NOx-soot → TE ~50%





Dual fuel with multiple injections - RCCI

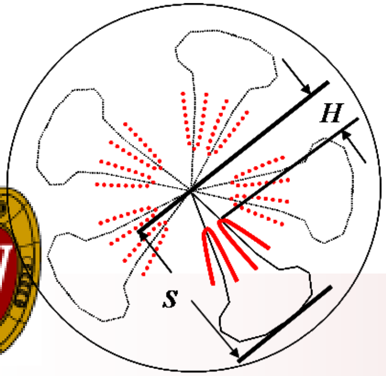


KIVA plus Genetic Algorithms used to optimize multiple injection strategy

Heavy- and light-duty ERC experimental engines

Engine	Heavy Duty	Light Duty
Engine	CAT SCOTE	GM 1.9 L
Displ. (L/cyl)	2.44	0.477
Bore (cm)	13.72	8.2
Stroke (cm)	16.51	9.04
Squish (cm)	0.157	0.133
CR	16.1:1	15.2:1
Swirl ratio	0.7	2.2
IVC (° ATDC)	-85 and -143	-132
EVO(° ATDC)	130	112
Injector type	Common rail	
Nozzle holes	6	8
Hole size (μm)	250	128

HD LD

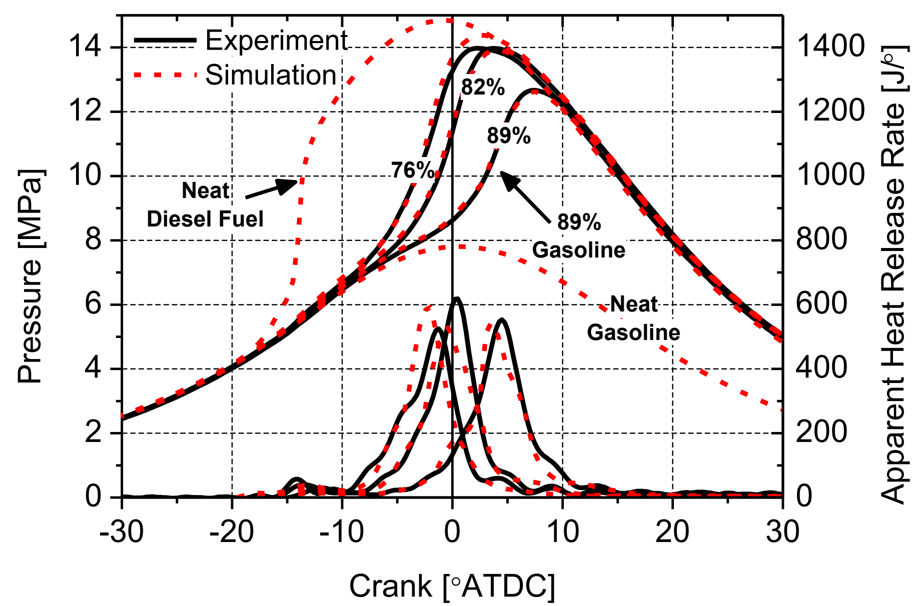


Engine size scaling
Staples et al.
SAE 2009-01-1124

RCCI experimental validation - HD Caterpillar SCOTE

IMEP (bar)	9		
Speed (rpm)	1300		
EGR (%)	43		
Equivalence ratio (-)	0.5		
Intake Temp. (° C)	32		
Intake pressure (bar)	1.74		
Gasoline (% mass)	76	82	89
Diesel inject press. (bar)	800		
SOI1 (° ATDC)	-58		
SOI2 (° ATDC)	-37		
Fract. diesel in 1st pulse	0.62		
IVC (°BTDC)/Comp ratio	143/16		

Effect of gasoline percentage

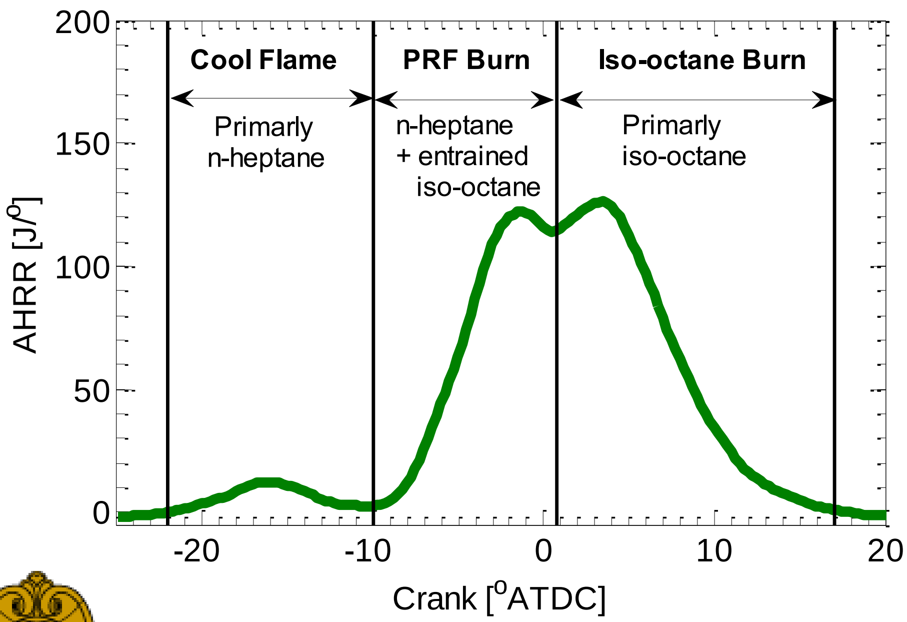


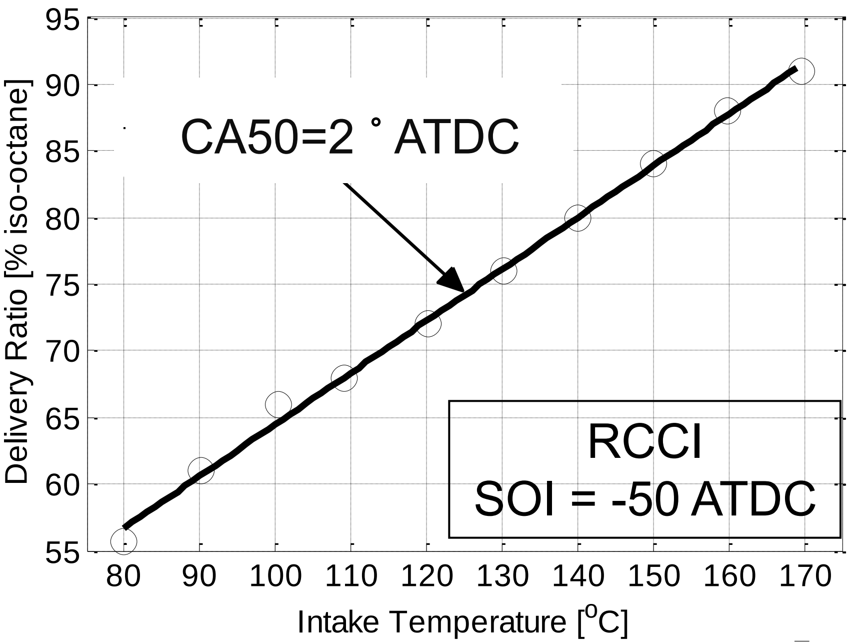
* Hanson et al.
SAE 2010-01-0864

- Computer modeling predictions confirmed
- Combustion timing and Pressure Rise Rate control with diesel/gasoline ratio
- Dual-fuel can be used to extend load limits of either pure diesel or gasoline

RCCI combustion – Controlled HCCI

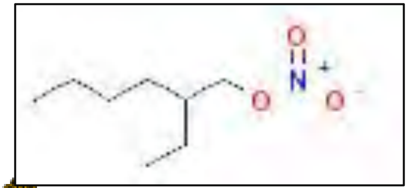
- Heat release occurs in 3 stages (SAE 2010-01-0345)
  - Cool flame reactions result from n-heptane (diesel) injection
  - First energy release occurs where both fuels are mixed
  - Final energy release occurs where lower reactivity fuel is located
- Changing fuel ratios changes relative magnitudes of stages
- Fueling ratio provides "next cycle" CA50 transient control

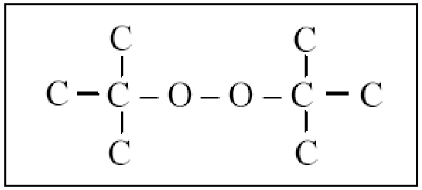


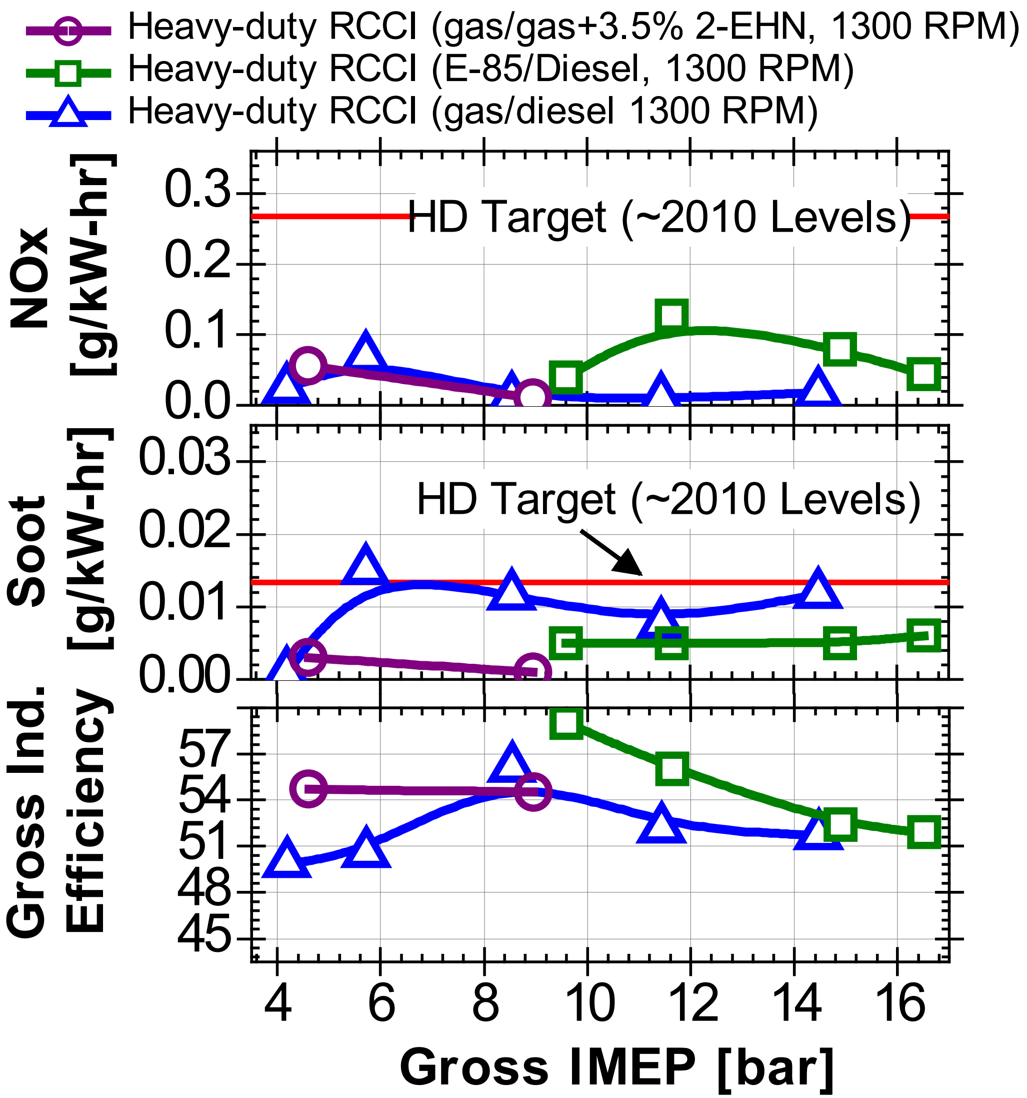


RCCI – high efficiency, low emissions, fuel flexibility

- Indicated efficiency of 59% achieved with E85/diesel
- Emissions met in-cylinder, without need for after-treatment
- Considerable fuel flexibility, including „single" fuel operation
- Diesel can be replaced with <0.5% total cetane improver (2-EHN/DTBP) in gasoline
  - less additive than SCR DEF
  - LD vehicle: windshield bottle-size every oil-change interval







Splitter et al. 2011-01-0363, Hanson et al. 2011-01-0361

Fuel flexibility and the future – renewable fuels

Reactivity Controlled Compression Ignition (RCCI) using Premixed Hydrated Ethanol and Direct Injection Diesel, Dempsey et al., ASME ICEF2011-60235

- Can RCCI be used with "wet" EtOH?

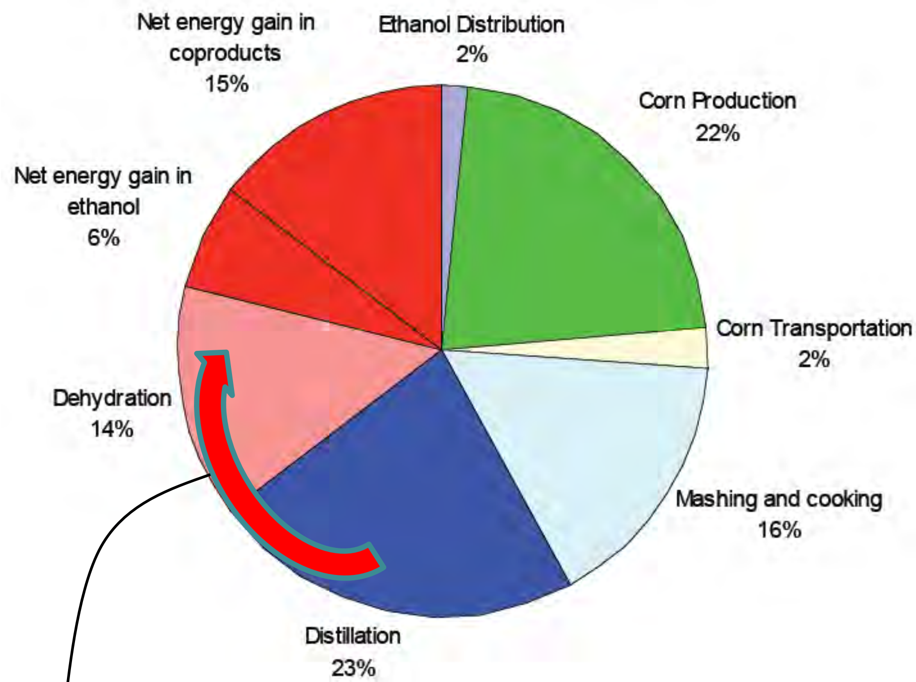
Cannot be used with SI engines due to lower flame speeds, misfire, condensation problems, phase separation of water with EtOH-gasoline

Cannot be used with diesel engines due to high EtOH octane number

Has been proposed for use in HCCI with intake heating – Berkeley, LLNL*

High heat of vaporization:

Gasoline=308, EtOH=924, H_2O=2400 kJ/kg

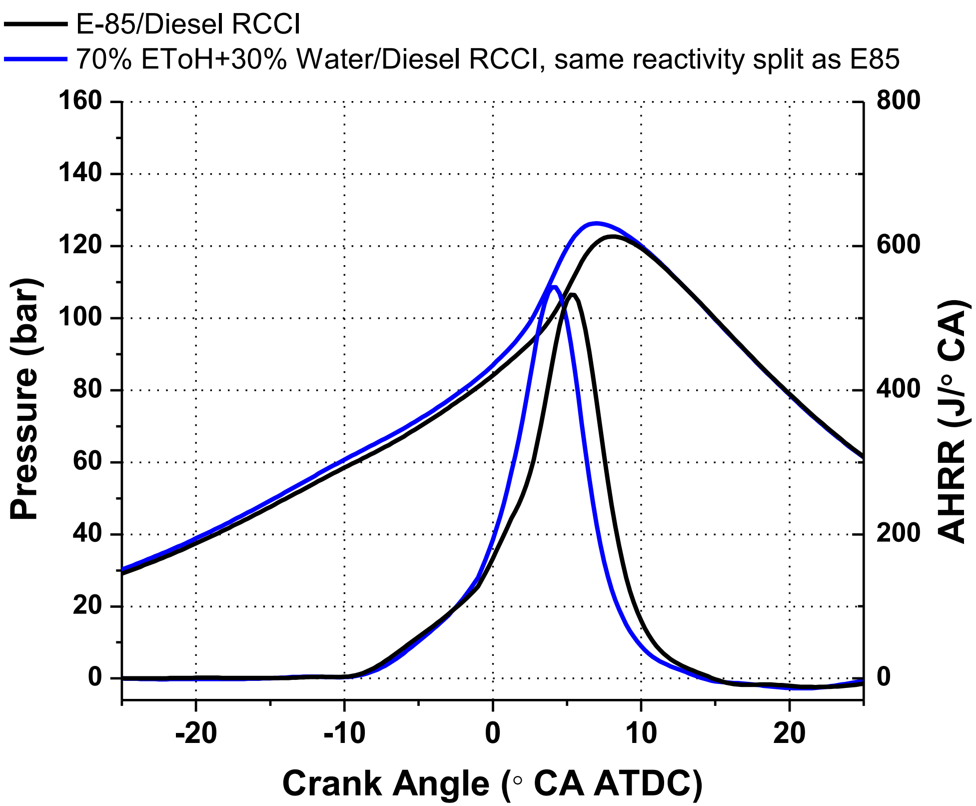


37% of fuel energy consumed in distillation-dehydration. Use of hydrated EtOH can give significant net energy gain

*Flowers et al. "Improving Ethanol Life Cycle Energy Efficiency by Direct Utilization of Wet Ethanol in HCCI Engines, SAE 2007-01-1867

Experimental results - Wet EtOH vs. E85 RCCI

ERC Caterpillar SCOTE

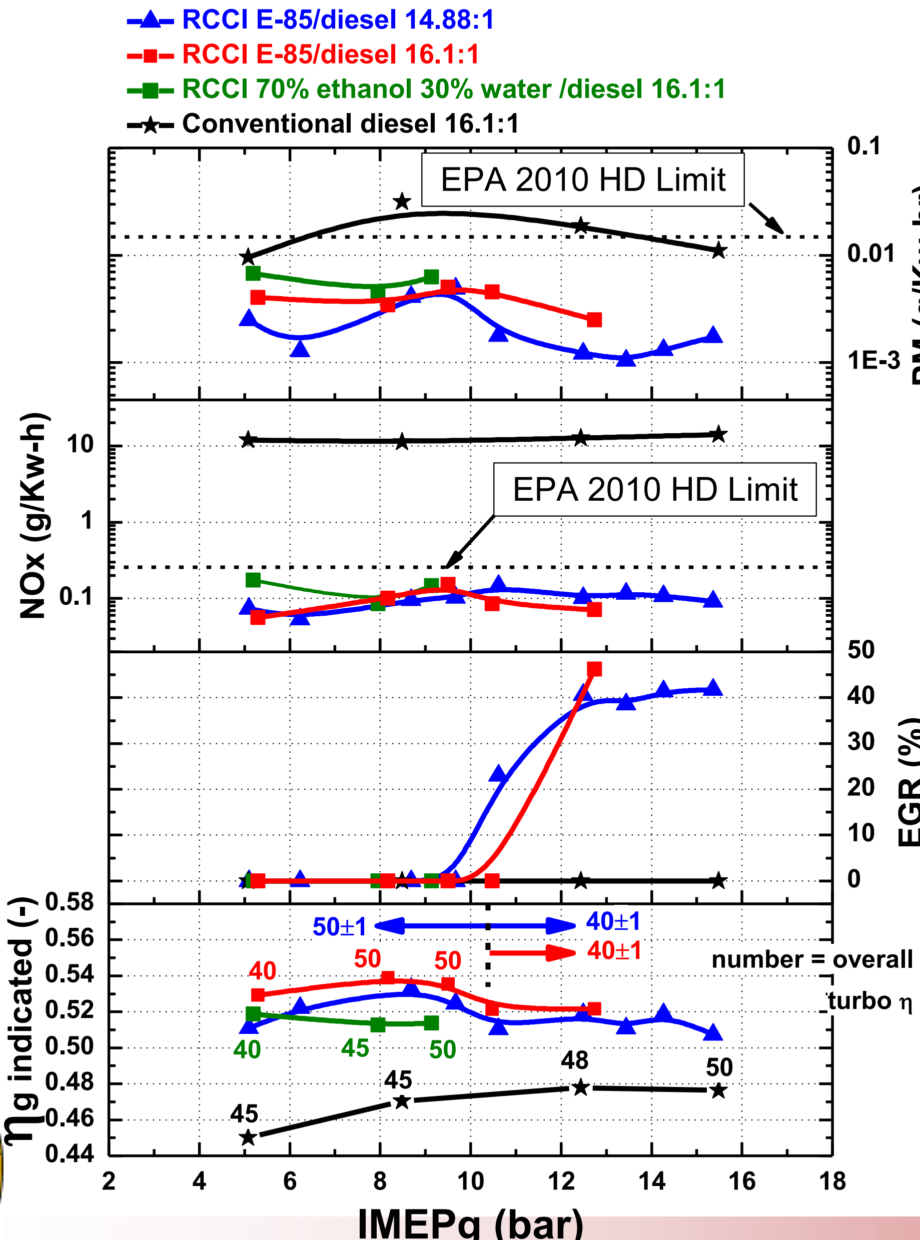


IMEPn	8.6	8.9
engine speed (rev/min)	1300	1300
Fuel 1	Wet EToH 70%	E85
Fuel 2	Diesel	Diesel
T Intake (°C)	54.8	35.5
fraction diesel	0.136	0.136
Φ (-) *	0.368	0.366
air flow (kg/min)	2.57	2.55
fuel energy (j/cycle)	4069	4082
η net (-)	0.483	0.507
CA50 (°CA ATDC)	3.8	4.6
RI (MW/m^2)	2.8	2.3
HC (g/kW-hr)	8.7	5.6
NOx (g/kW-hr)	0.148	0.148
CO (g/kW-hr)	5.6	5.7
PM (g/kW-hr)	0.0063	0.0041
EGR (%)	0.0	0.0

* Φ calculated from EToH and Diesel only, water fraction ignored

- Combustion event nearly identical to E85/diesel RCCI
- +20°C intake temperature with wet EtOH to maintain combustion phasing

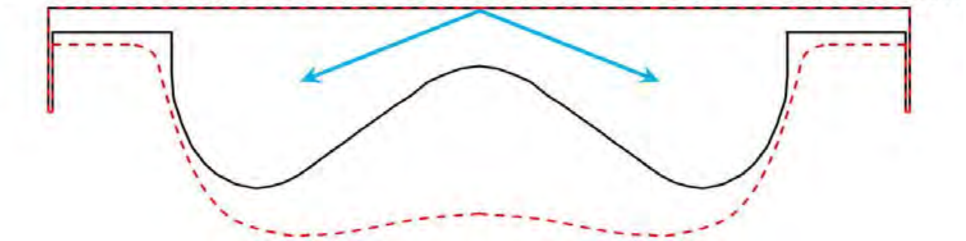
Comparison of Wet EtOH & E85 RCCI vs. diesel



- Hydrous EtOH efficiency between conventional diesel and E85 RCCI
- Standard diesel gross thermal efficiency ~3-4 points lower than Hyd. EtOH, which is ~1-3 points lower than E85
- Hydrous EtOH has increased combustion losses (+~1%)
- EtOH and E85 RCCI NOx & PM emissions nearly identical
- Conventional diesel NOx two orders higher than EtOH or E85 RCCI

Optimization of piston geometry for RCCI

Computational Optimization of Reactivity Controlled Compression Ignition in a Heavy-Duty Engine with Ultra Low Compression Ratio – SAE 2011-24-0015



Operating Conditions	Low-Load	Mid-Load	High-Load
Speed [rpm]	800	1300	1800
Fuel [mg/cycle]	48	94	270
Gross IMEP [bar]	~ 4	~ 9	~ 23
Intake Temp. [C]	60	60	60
Intake Press. [bar abs.]	1.0	1.75	3.0

Design Parameter			
Premixed Gasoline [%]	10 to 95	30 to 95	60 to 95
DI Diesel SOI #1 [ATDC]	-100 to -50	-100 to -50	-100 to -30
DI Diesel SOI #2 [ATDC]	-40 to 0	-40 to 0	-15 to 10
Diesel Fuel in 1st Inj. [%]	0 to 100	0 to 100	0 to 100
Diesel Inj. Press. [bar]	300 to 1500	300 to 1500	300 to 1500
EGR [%]	0 to 60	0 to 60	0 to 50

CFD with NSGAII Optimization:
ISFC, NOx, Soot, CO, UHC, PPRR

KIVA 3v release 2 code
CHEMKIN II - 42 species
ERC PRF mechanism

Fuel	Chemistry	Spray
Gasoline	iso-octane	iso-octane
Diesel fuel	n-heptane	tetradecane

RANS model (RNG k-ε)

KH-RT spray breakup model

Gasjet spray model
Reduced grid dependency for droplet drag calculations in near nozzle region

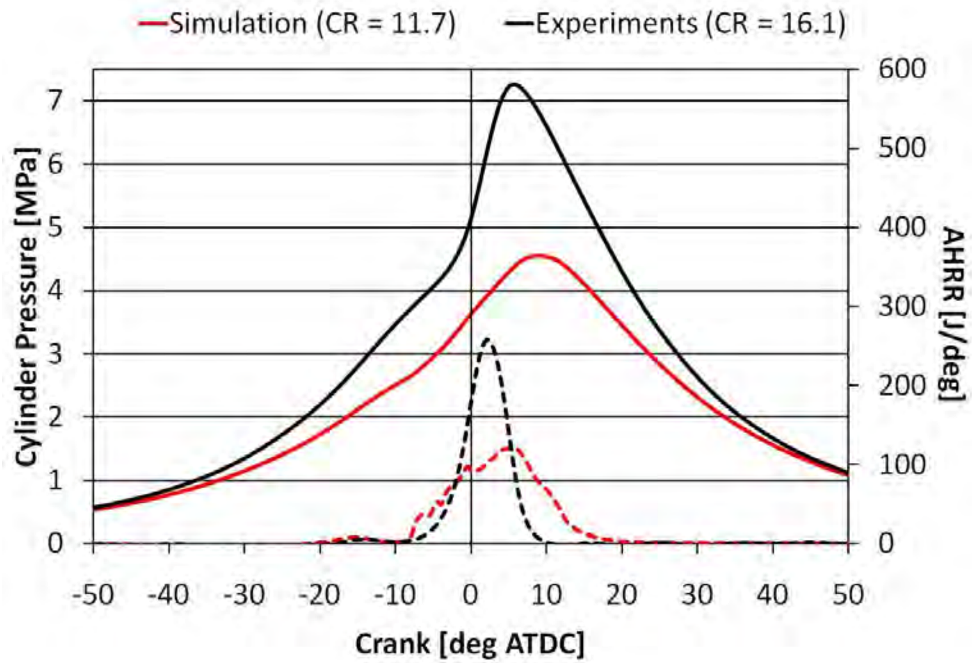
Light-Load (~4 bar IMEP) CR=11.7 results

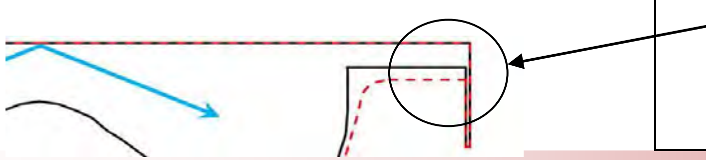
Design Parameter		CR=11.7 Simulated	CR=16.1 Experiments
Total Fuel	[mg/cycle]	48	53
Engine Speed	[rpm]	800	800
Gasoline	[%]	77%	81%
Diesel SOI #1	[ATDC]	-60.5	-62.0
Diesel SOI #2	[ATDC]	-39.2	-37.0
Diesel in 1st Inj.	[%]	39%	70%
Diesel Inj. Press.	[bar]	1432	400
EGR	[%]	0%	0%
Equivalence Ratio	[-]	0.29	0.32
Intake Pressure	[bar abs.]	1.00	1.03
Exhaust Pressure	[bar abs.]	1.05	1.07

***Net Cycle Results**

NOx	[g/ikW-hr]	0.11	0.02
Soot	[g/ikW-hr]	0.009	0.001
CO	[g/ikW-hr]	4.0	7.0
UHC	[g/ikW-hr]	2.6	8.0
ISFC	[g/ikW-hr]	170.8	174.7
$\eta_{thermal}$	[%]	48.8%	47.7%
PPRR	[bar/deg]	1.5	5.3

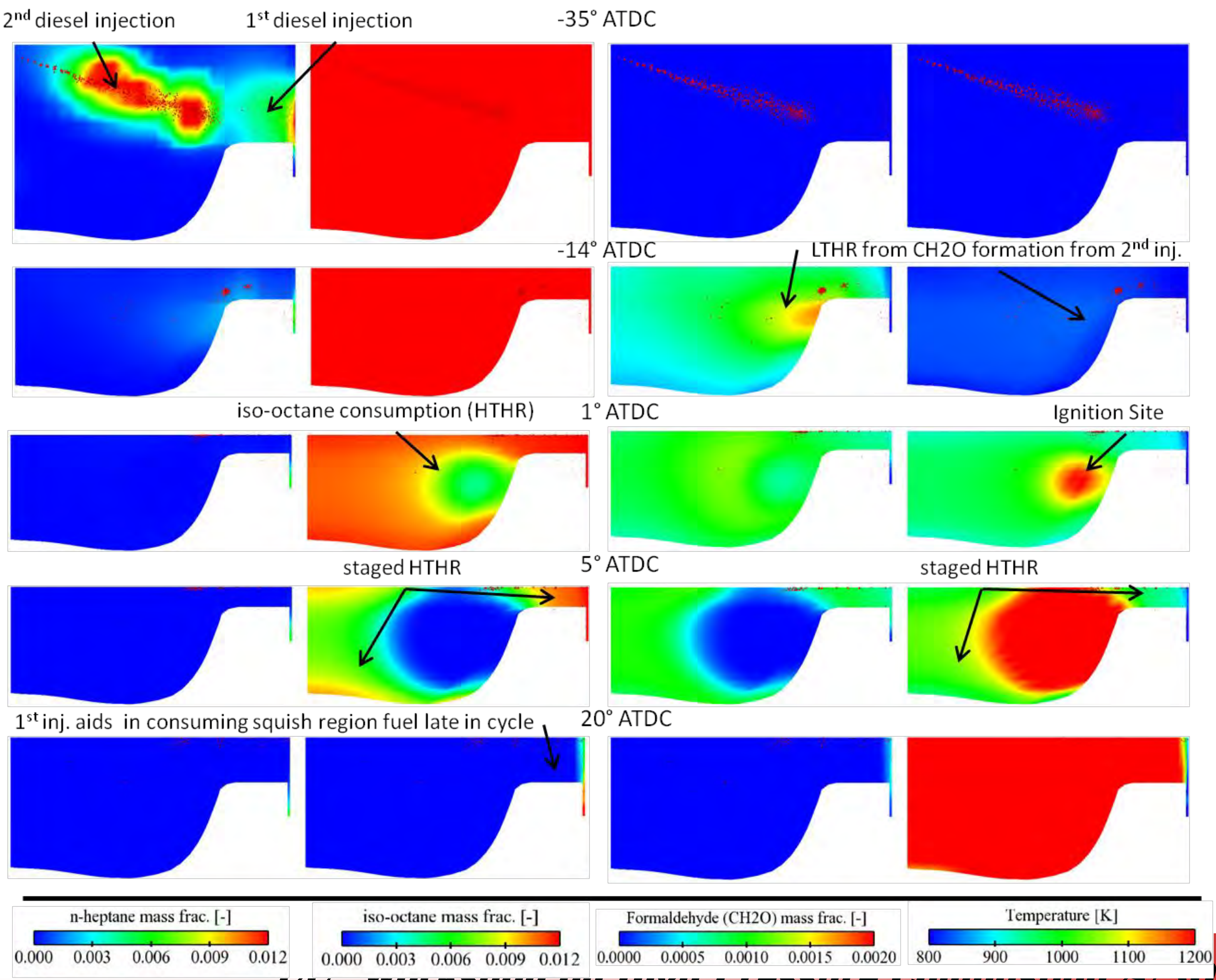
* -360° to 360° ATDC cycle. Simulated pumping loop obtained from 1D cycle simulation





- Results compared with CR=16.1 experimental data (SAE 2011-01-0363)
- Combustion efficiency is improved with lower compression ratio due to smaller top ring land (reduced CO/UHC) and more reactive fuel amount

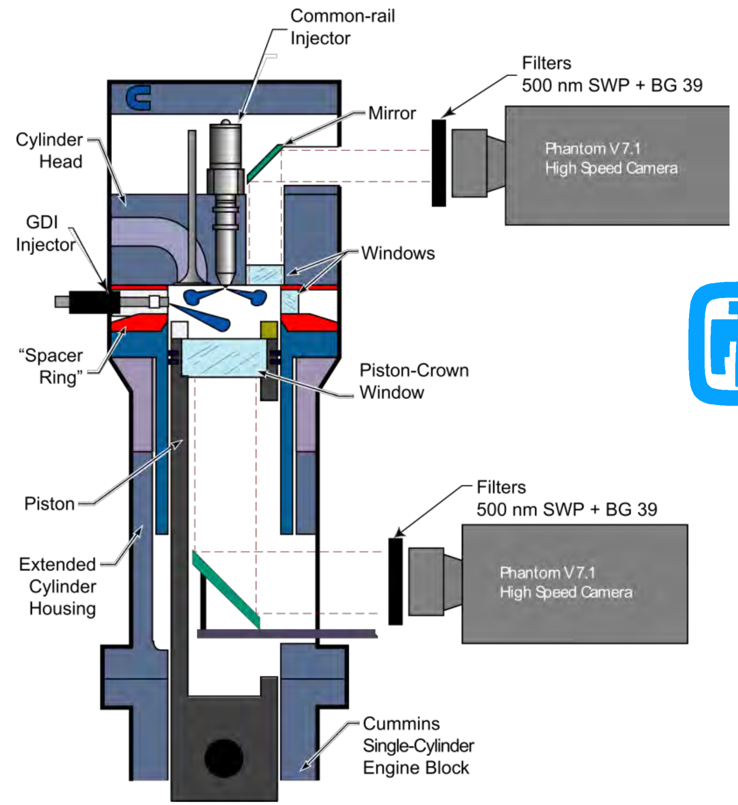
Light-Load combustion characteristics

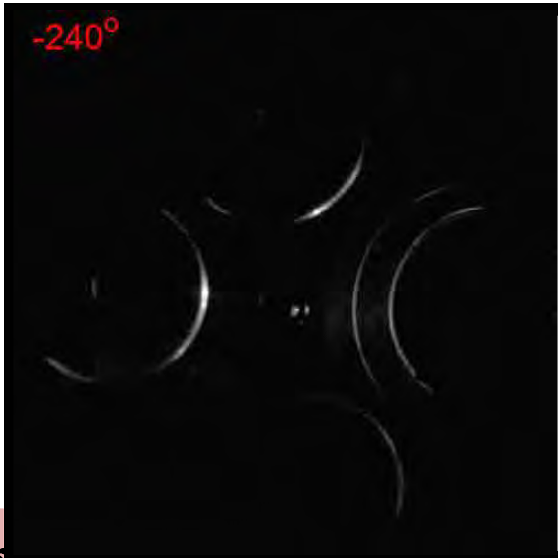


RCCI optical experiments

Engine	Cummins N-14
Bore x stroke	13.97 x 15.24 cm
Displacement	2.34 L
Geometric compression ratio	10.75

- RCCI experiments in Sandia heavy-duty optical engine
- LED illumination through side windows to visualize sprays
- Images recorded through both piston-crown and upper window
- Crank-angle-resolved high-temperature chemiluminescence with high-speed CMOS camera
- Short-wave pass filter to reject long-wavelength (green through IR) soot luminosity





GDI
Iso-octane
100 bar
7x150 micron

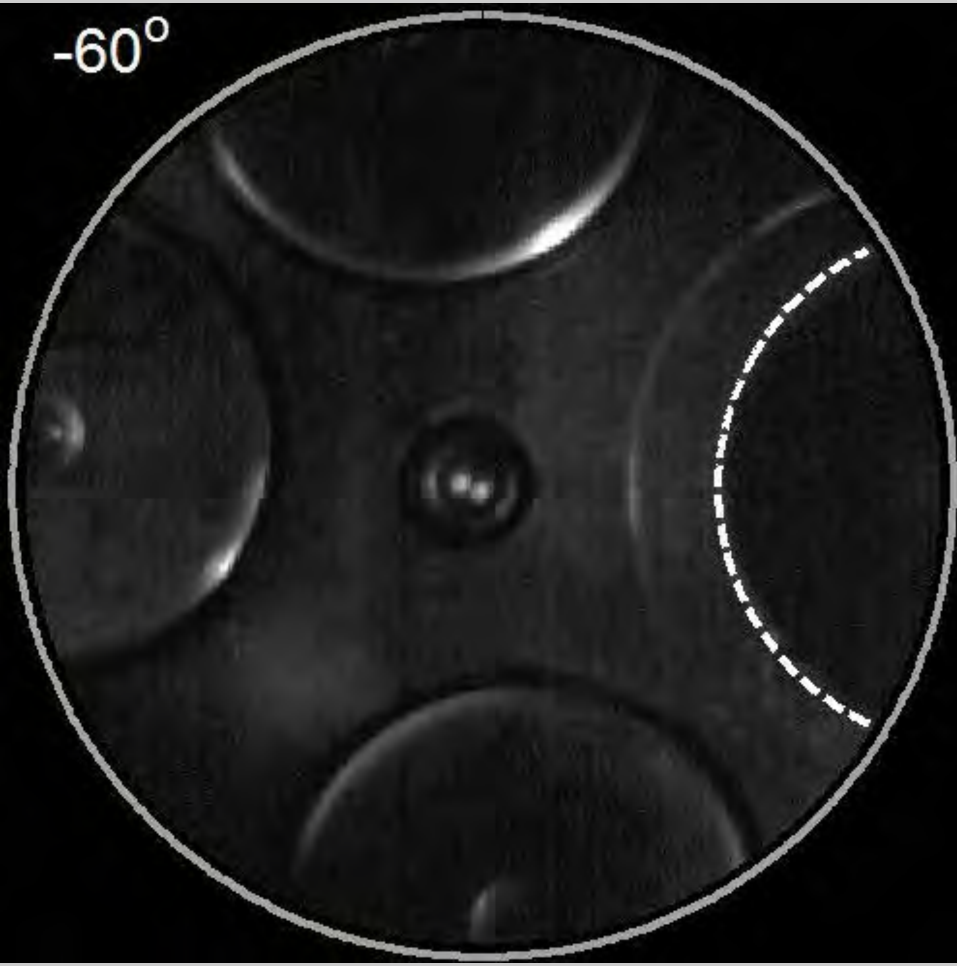
Common-rail
n-heptane
600 bar
8x140 micron
Inc. Ang. 152°

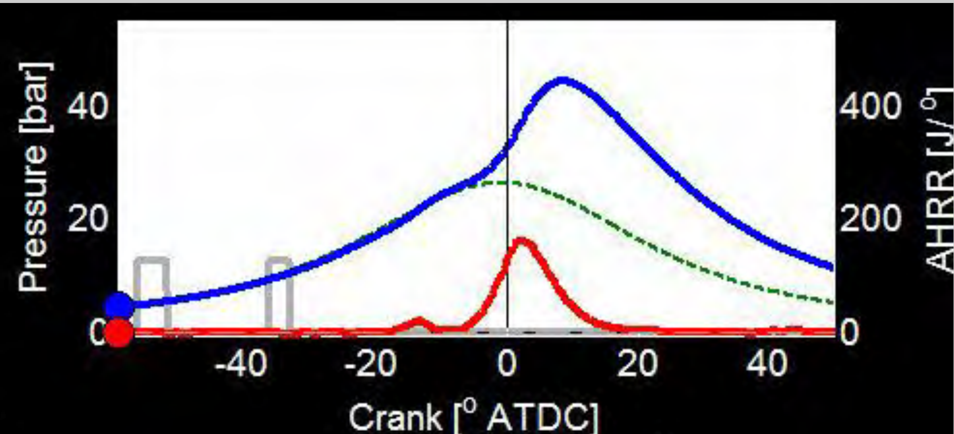
RCCI high speed combustion luminosity imaging

Load:	4.2 bar IMEP
Speed:	1200 rpm
Intake Temperature:	90° C
Intake Pressure:	1.1 bar abs.

Kokjohn, S.
Musculus, M.P.B
Reitz, R.D.,
ILASS-2011

GDI SOI:	-240°ATDC
CR SOI:	-57°/-37° ATDC
Equivalence ratio:	0.42
Iso-octane mass %:	64



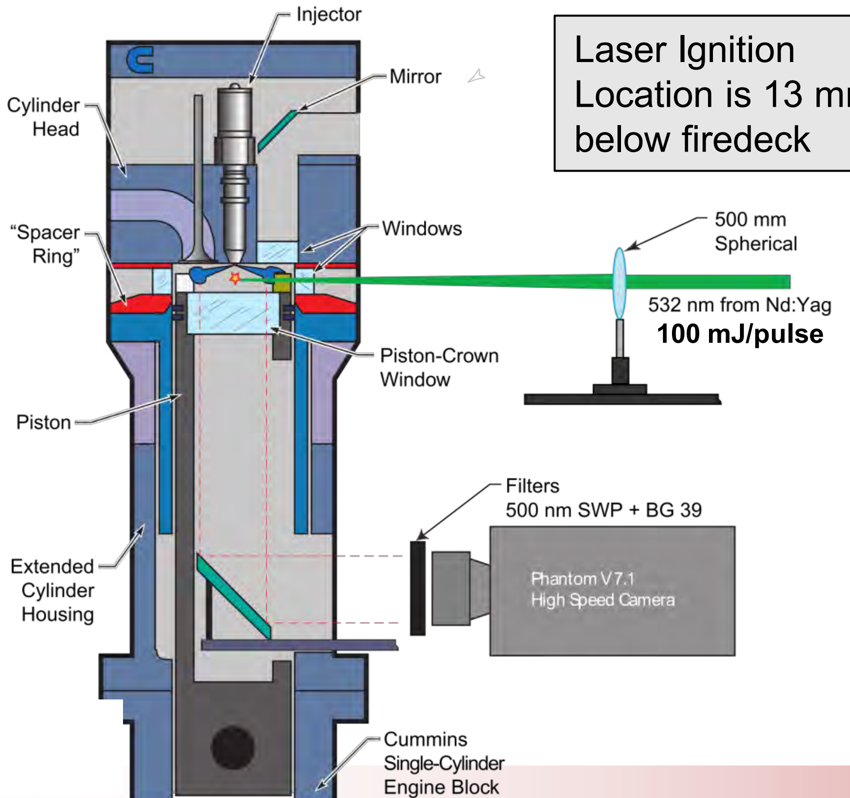


Bowl window

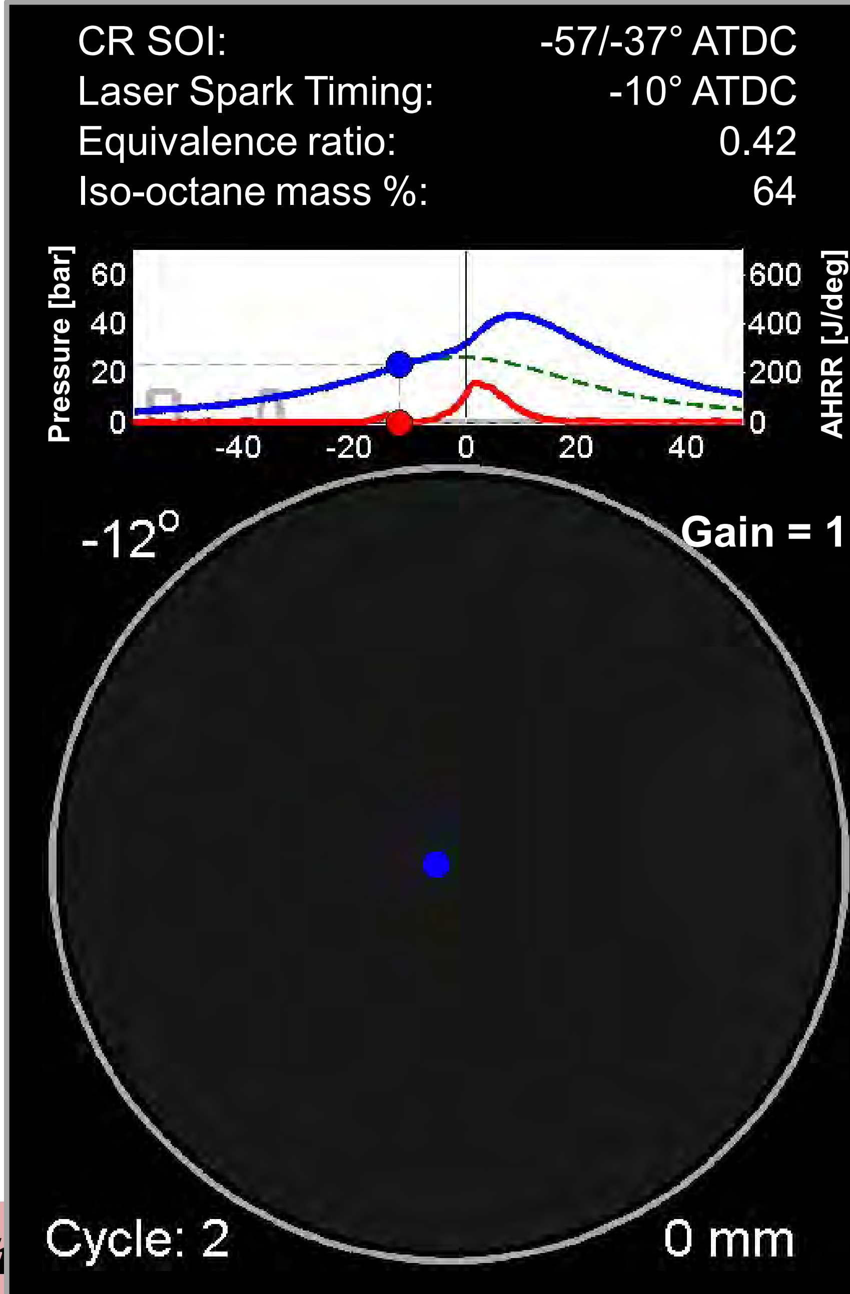
Squish (upper) window

RCCI – Combustion mechanisms

- CFD and toluene fluorescence experiments show that reaction zone growth follow gradients in fuel reactivity → mechanism of growth is still unclear
- Laser ignition is used to probe ignitability throughout the chamber

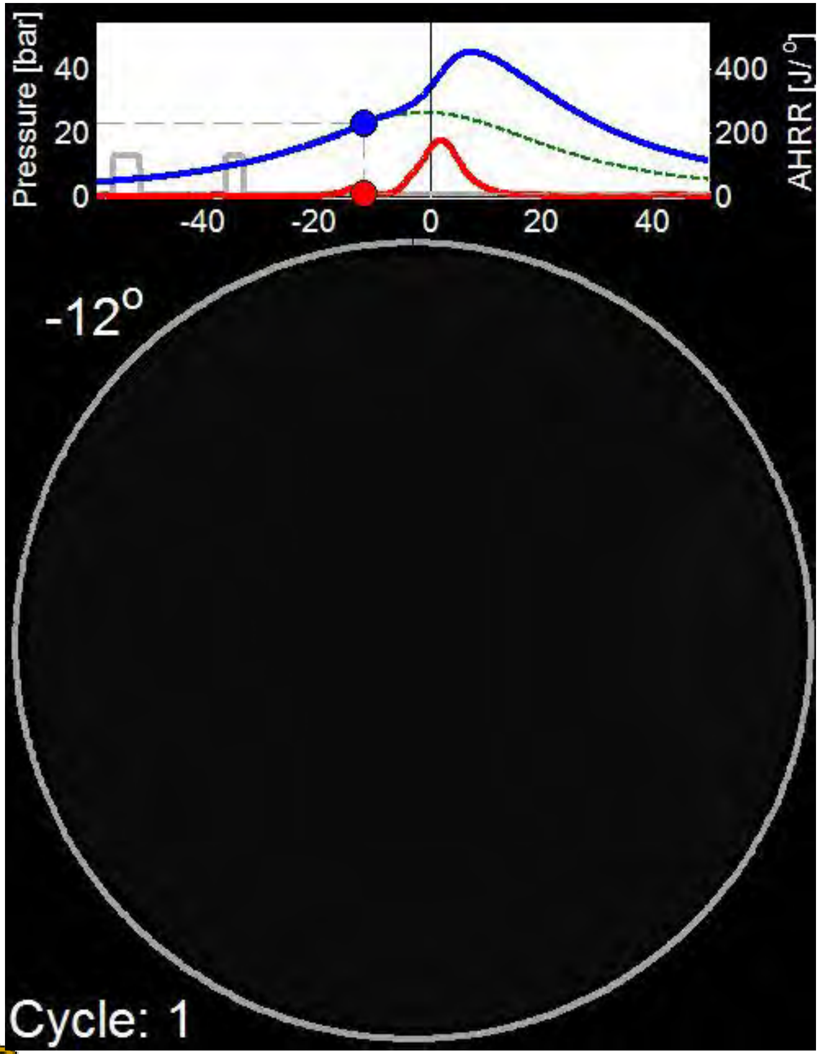


Laser Ignition Location is 13 mm below firedeck

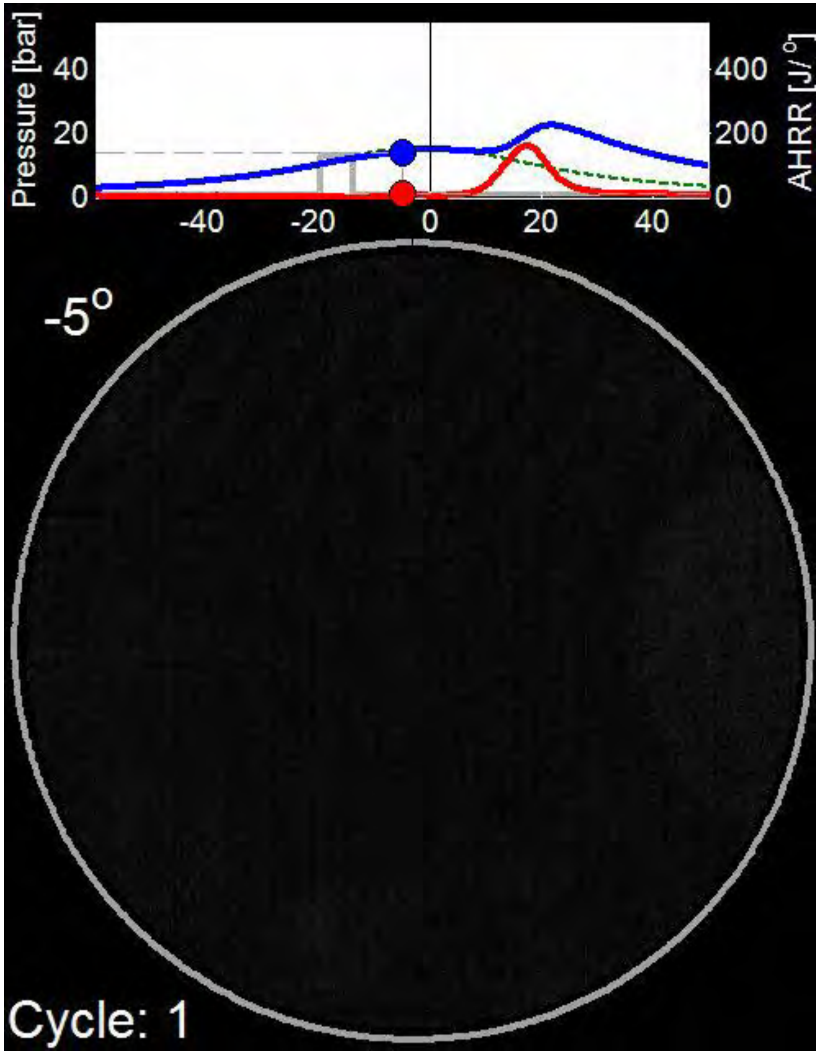


RCCI – flame propagation or volumetric ignition?

Laser ignition 67 mJ pulse 30 mm from injector and 13 mm below firedeck



Phi=0.42



Phi=0.8

CFD model considering flame propagation

KIVA-CHEMKIN-G code

- CHEMKIN based chemistry solver used for ignition and volumetric heat release
  - Each cell considered a well-stirred reactor (WSR)
  - ERC reduced PRF mechanism
- Level set based model (G-equation) for turbulent flame propagation
  - Modeling approach has been validated over a wide range of conditions in gasoline direct-injection engines (Yang et al. SAE 2008-01-2391)
  - Damköhler number is used to select the combustion regime for flame containing cells

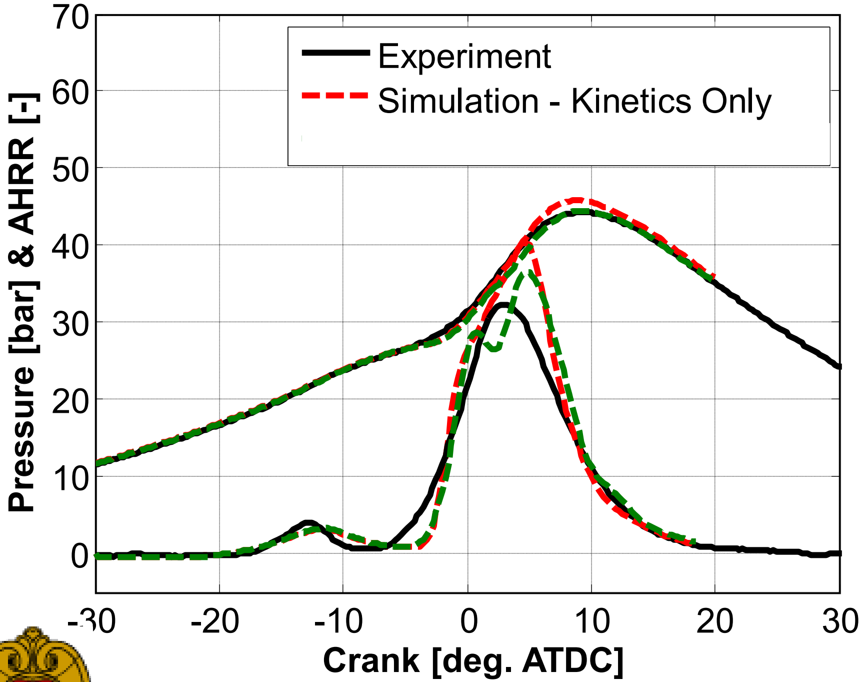
$$\mathrm{Da} = \frac{\tau_{lam}}{\tau_{chem}} = \frac{\delta_l / S_l}{\tau_{chem}}$$

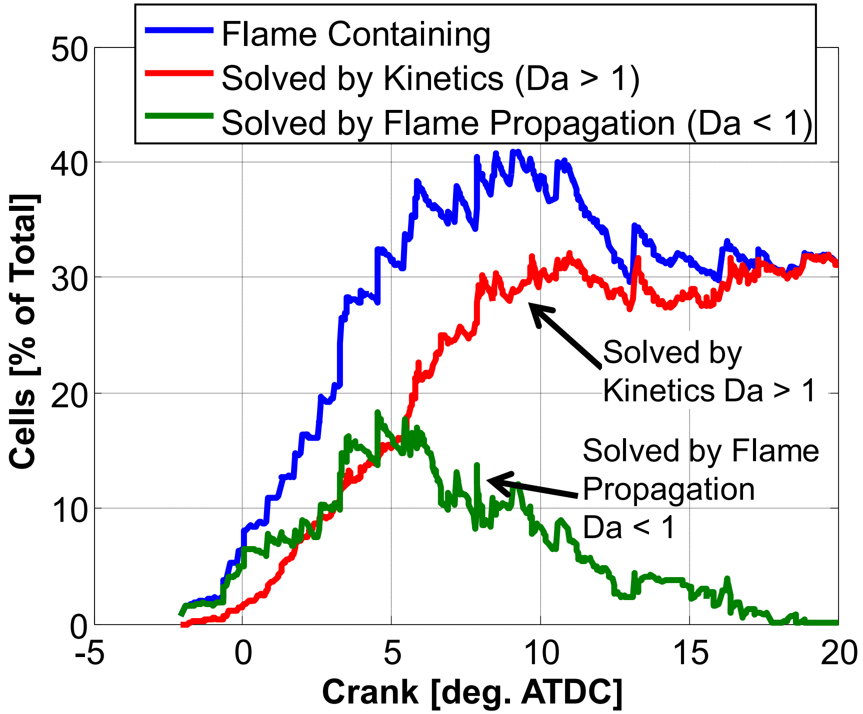
$$\mathrm{Da} > 1 \qquad \text{Kinetics Solution}$$

$$\mathrm{Da} < 1 \qquad \text{Flame Propagation}$$

CFD model considering flame propagation

- Modeling results without consideration of flame propagation show reasonable agreement with measured cylinder pressure and AHRR
- Considering flame propagation (G-equation model) results in minor changes in the energy release
- Initially, the small number of flame containing cells are dominated by flame propagation.





Full-Load (~23 bar IMEP) CR=11.7 – low emissions

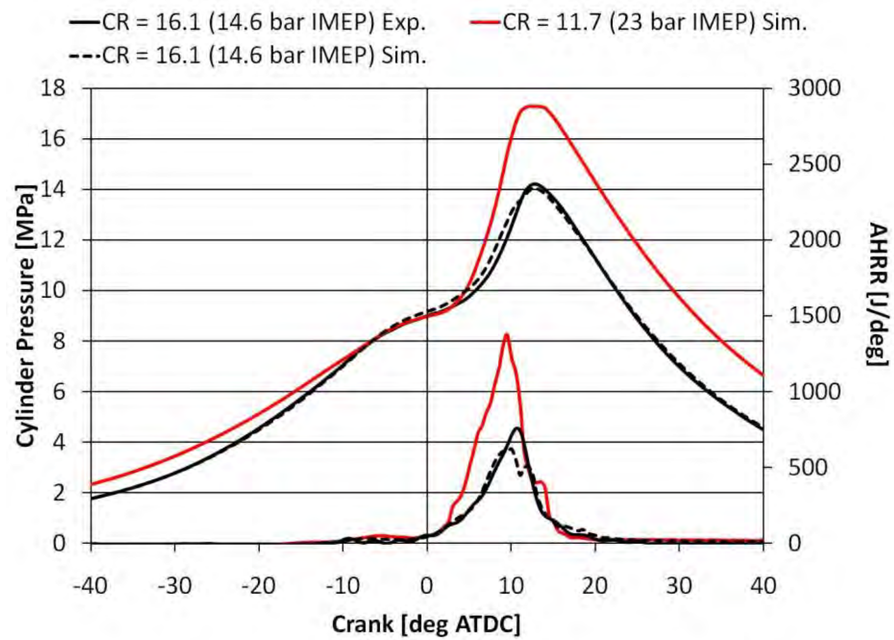
Design Parameter		***CR=11.7 Simulated***	***CR=16.1 Experiment (14.6 bar)***
Total Fuel	[mg/cycle]	270	161
Engine Speed	[rpm]	1800	1300
Gasoline	[%]	87%	90%
Diesel SOI #1	[ATDC]	-49.1	-58.0
Diesel SOI #2	[ATDC]	-4.5	-37.0
Diesel in 1st Inj.	[%]	72%	37%
Diesel Inj. Press.	[bar]	1450	800
EGR	[%]	42%	57%
Equivalence Ratio	[-]	0.93	0.97
Intake Pressure	[bar abs.]	3.00	2.34
Exhaust Pressure	[bar abs.]	3.15	2.52

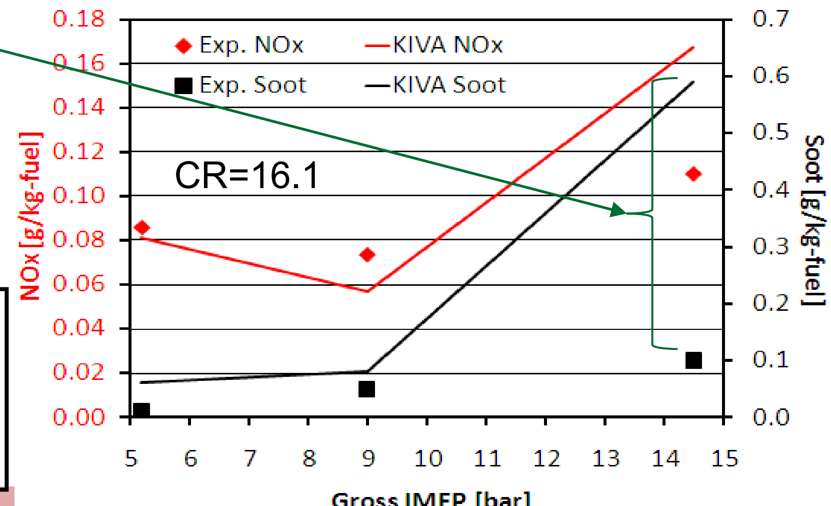
****Net Cycle Results***		***CR=11.7 Simulated***	***CR=16.1 Experiment***	***CR=16.1 Simulated***
NOx	[g/ikW-hr]	0.30	0.02	*0.03*
Soot	[g/ikW-hr]	0.093	0.016	*0.089*
CO	[g/ikW-hr]	5.8	12.4	*8.4*
UHC	[g/ikW-hr]	1.2	1.9	*2.7*
ISFC	[g/ikW-hr]	178.8	168.5	*163.8*
$\eta_{thermal}$	[%]	46.6%	49.5%	*50.8%*
PPRR	[bar/deg]	15.5	9.4	*8.0*

* -360° to 360° ATDC cycle. Simulated pumping loop obtained from 1D cycle simulation

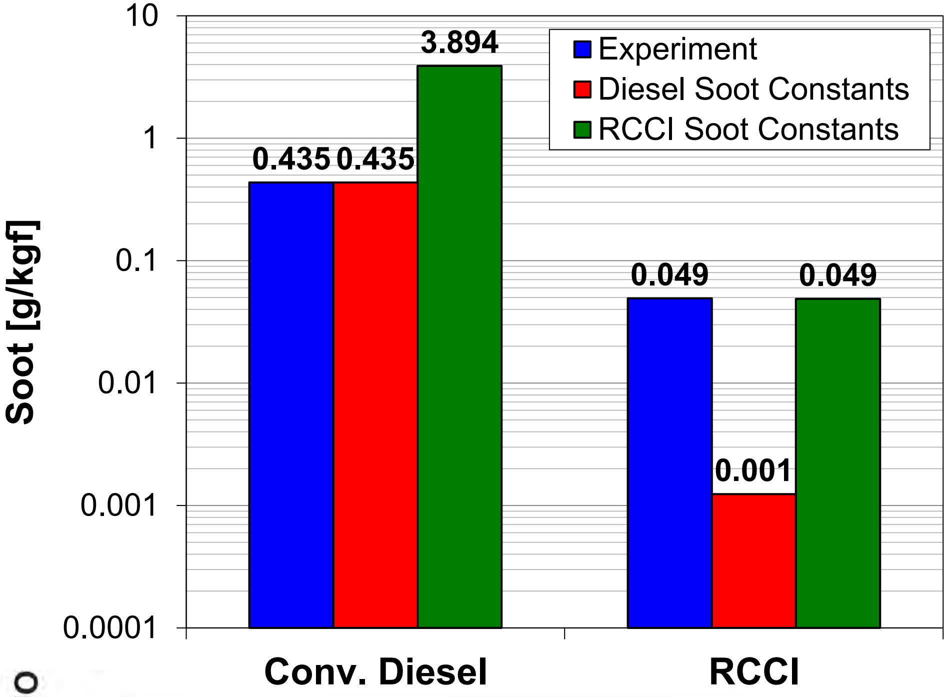
- Full load RCCI achievable with low CR piston

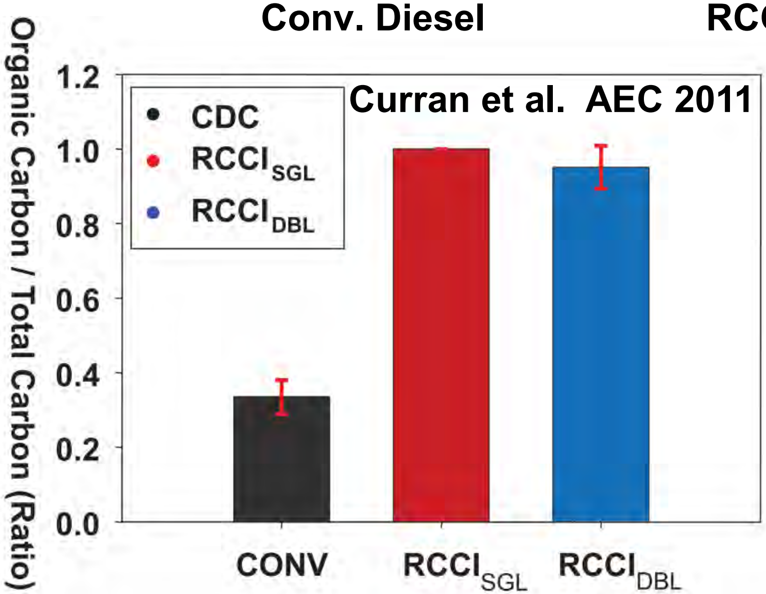
- Soot model constants uncertain for globally stoichiometric RCCI: soot emissions over-predicted

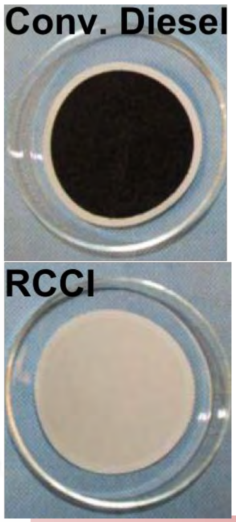




RCCI Soot Modeling







Two-step soot model

Soot formation rate

$$\frac{dM_{sf}}{dt} = A_{sf} M_{C_2H_2} P^{0.5} \exp\left(-E_{sf}/RT\right)$$

	Asf (s^{-1}-$bar^{-0.5}$)	Esf (cal/mol)
Diesel soot constants	1,000	12,500
RCCI soot constants	700	1,250

- Very different soot model constants required for conventional diesel and RCCI combustion
- ORNL experiments show soot composition is dependent on operating condition
  - Conventional diesel soot is ~30% organic carbon
  - RCCI soot is greater than 90% organic carbon

Conclusions and future research directions

RCCI offers practical low-cost pathway to >15% improved diesel engine fuel efficiency (lower CO_2) + meet emission mandates in-cylinder

Inconvenience of two fuels already accepted by diesel industry (diesel/urea)

RCCI is cost effective:

- low cost port-injected less reactive fuel (e.g., gasoline, E85, "wet" EtOH, C/LNG) with optimized* low pressure DI of more-reactive fuel (e.g., diesel/additized gas)
- Diesel or GDI (w/spark plug) operation can be retained (limp home).

RCCI offers great fuel flexibility and transient control:

- proportions of low and high reactivity fuels can be changed dynamically, based on fuels used with same/next-cycle combustion feedback control

Further RCCI research requires fundamental studies of:

- Chemical kinetic mechanisms for realistic fuels and additives (e.g., EHN, DTBP)
- Mixed combustion regimes: flame propagation vs. volumetric heat release
- Soot models for LTC regimes with low organic carbon fraction – fuel effects

Further RCCI engine development requires R&D:

- Engine feedback control, load extension (e.g., via: multiple injections, CR, VVA), optimized combustion chamber geometry, boost pressure, EGR, charge-air cooling, fuel effects (LNG), etc.

* WARF Pat. pending

Thank you for your attention!