Reciprocating Internal Combustion Engines

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2014 Princeton-CEFRC
Summer School on Combustion
Course Length: 15 hrs

(Mon.- Fri., June 23 – 27, 2014)

Short course outine:

Engine fundamentals and performance metrics, computer modeling supported by in-depth understanding of fundamental engine processes and detailed experiments in engine design optimization.

Day 1 (Engine fundamentals)
- Part 1: IC Engine Review, 0, 1 and 3-D modeling
- Part 2: Turbochargers, Engine Performance Metrics

Day 2 (Combustion Modeling)
- Part 3: Chemical Kinetics, HCCI & SI Combustion
- Part 4: Heat transfer, NOx and Soot Emissions

Day 3 (Spray Modeling)
- Part 5: Atomization, Drop Breakup/Coalescence
- Part 6: Drop Drag/Wall Impinge/Vaporization/Sprays

Day 4 (Engine Optimization)
- Part 7: Diesel combustion and SI knock modeling
- Part 8: Optimization and Low Temperature Combustion

Day 5 (Applications and the Future)
- Part 9: Fuels, After-treatment and Controls
- Part 10: Vehicle Applications, Future of IC Engines

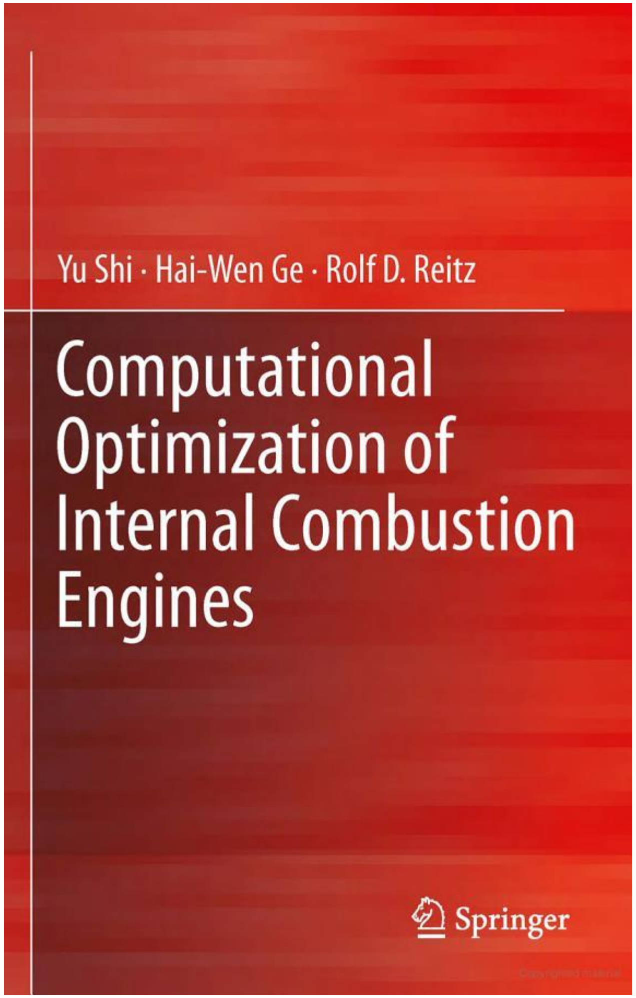
Overview of optimization techniques

- Enumerative or exhaustive
- Calculus or gradient-based

  "local" methods which search in the neighborhood of current design point
- Random

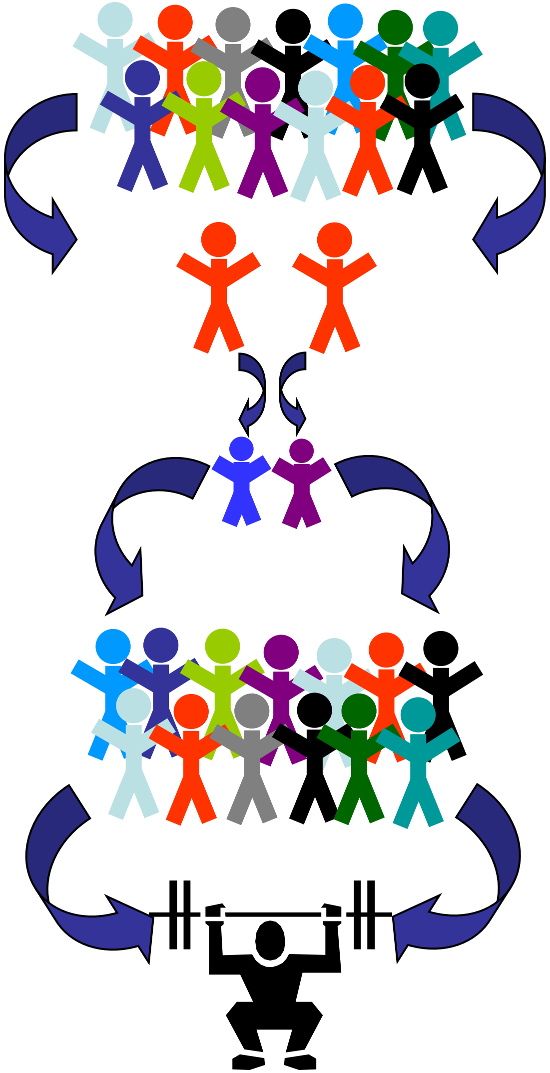
  "global" methods such as genetic algorithms (GA) which typically converge on a global optimum
- Univariate (one-factor-at-a-time)
- Design of Experiments (DOE)

  Two-level factorial designs (main and interaction effects)
  Response surface methods (RSM)
  Statistical model building



Senecal, 2000

Genetic algorithms



"Individuals" are generated through random selection and a "population" is produced

A model is used to evaluate the fitness of each individual

The fittest individuals are allowed to "reproduce"

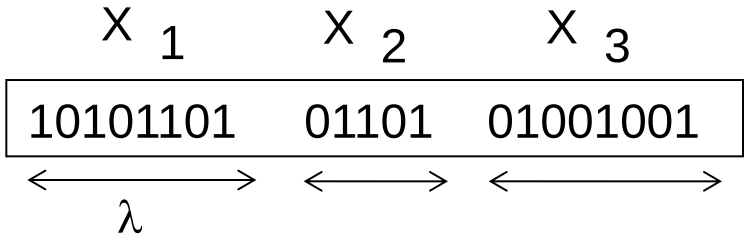
A new "generation" is formed - "mutations" are allowed through random changes

The fitness criteria thins out the population and the most fit solution is achieved over successive generations

Goldberg, 1989
Carrol, 1996
Senecal, 2000

Implementation of algorithm

Binary representation of parameters X - “genes”

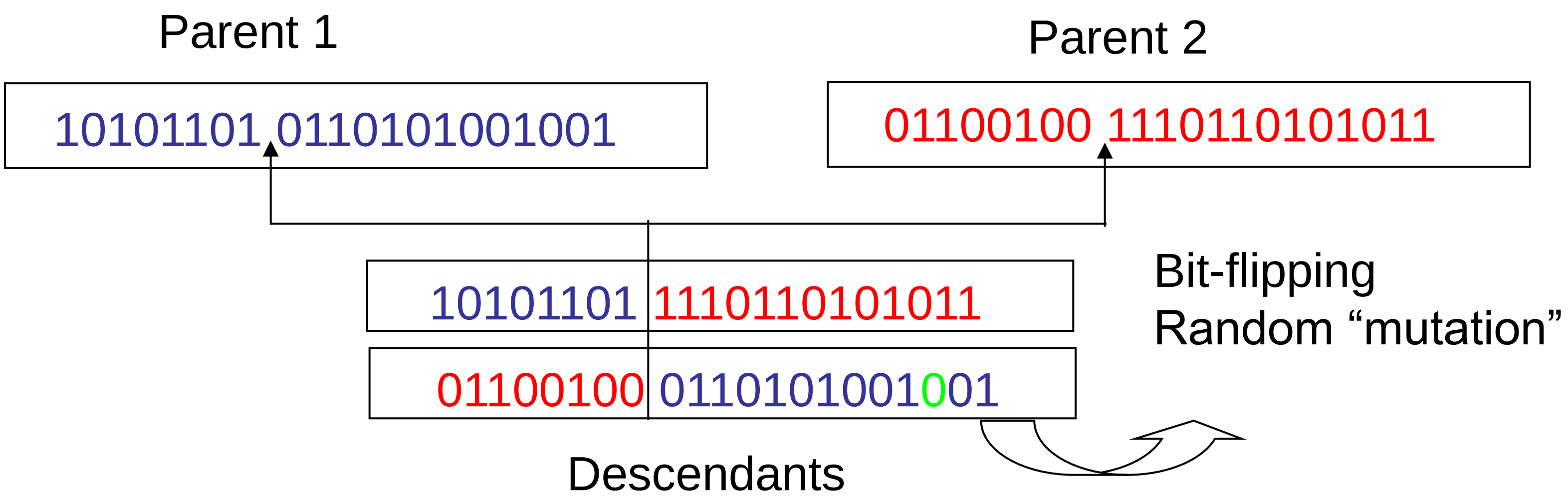


10101101 01101 01001001 - “chromosome” gene string

Precision $$\pi = \frac{X_{i,\max} - X_{i,\min}}{2^{\lambda} - 1}$$

Evaluate merit *f* (X) for each generation member - identify “fittest”

Binary tournament selection → Bit-swapping “Cross-over”



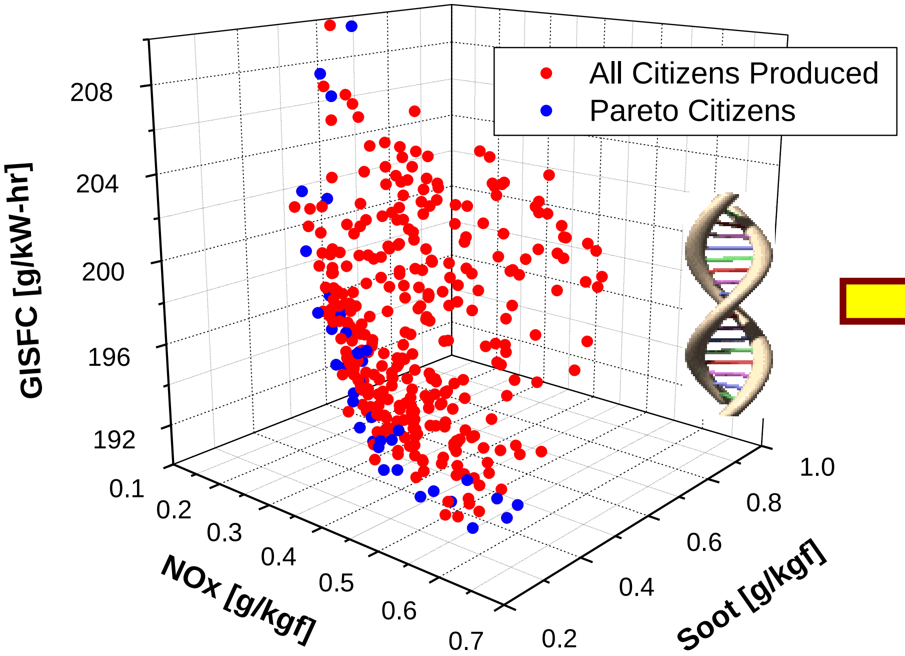
Bit-flipping
Random “mutation”

Liu, 2006

Coello, 2001

Optimization methodology

Multi-Objective Genetic Algorithm



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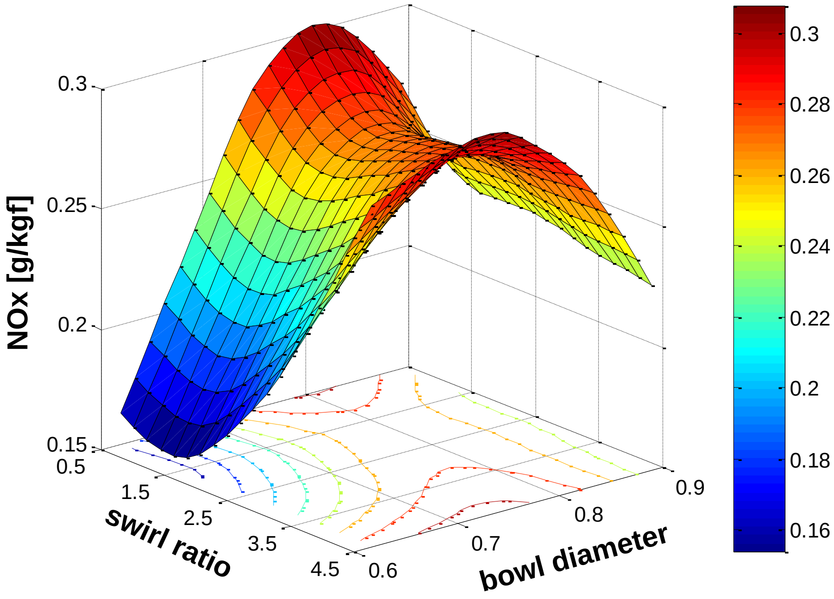
Nonparametric Regression Technique



Simultaneous optimization of many objectives [1]

No merit function required to drive search

Pareto front offers more information than a single optimum

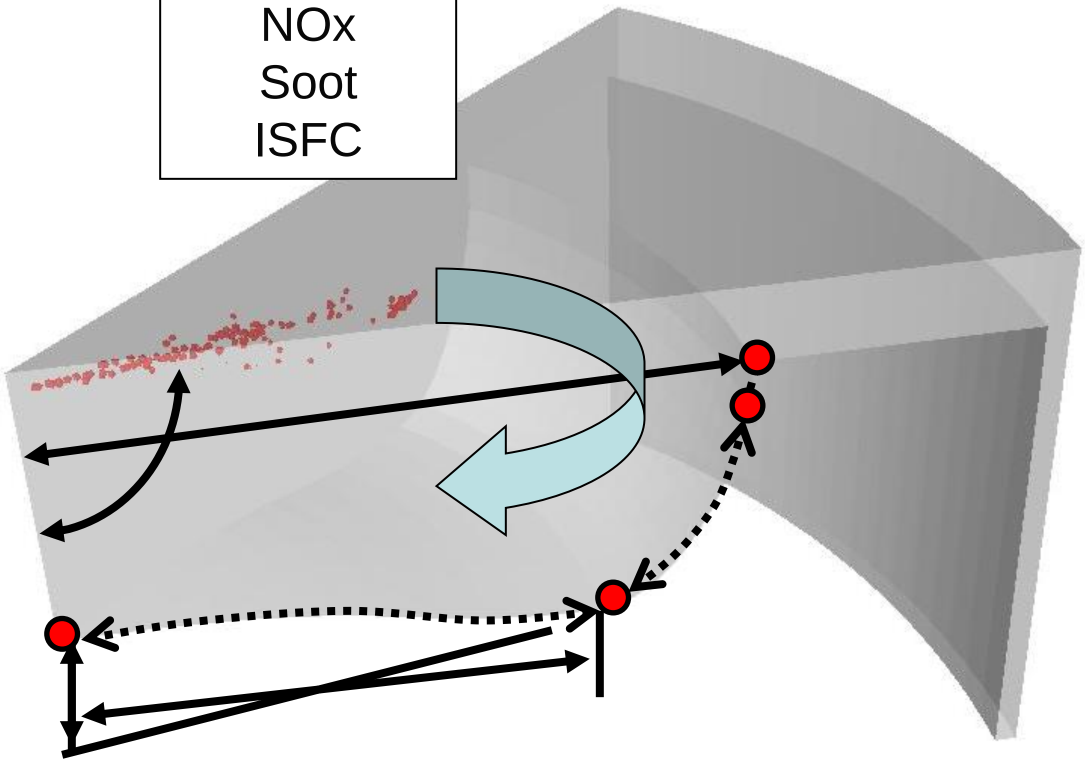
Regression technique suitable for handling irregular and undesigned data sets (e.g., GA data) [2]

Utilizes otherwise discarded optimization data

Captures magnitude of effects AND the shape of their response

Example optimization - piston bowl design

Parameters and Objectives



Optimize:
NOx
Soot
ISFC

7 Geometry Parameters:

Pip height

Bowl diameter

ϕ of bowl bottom

4 curvature control points

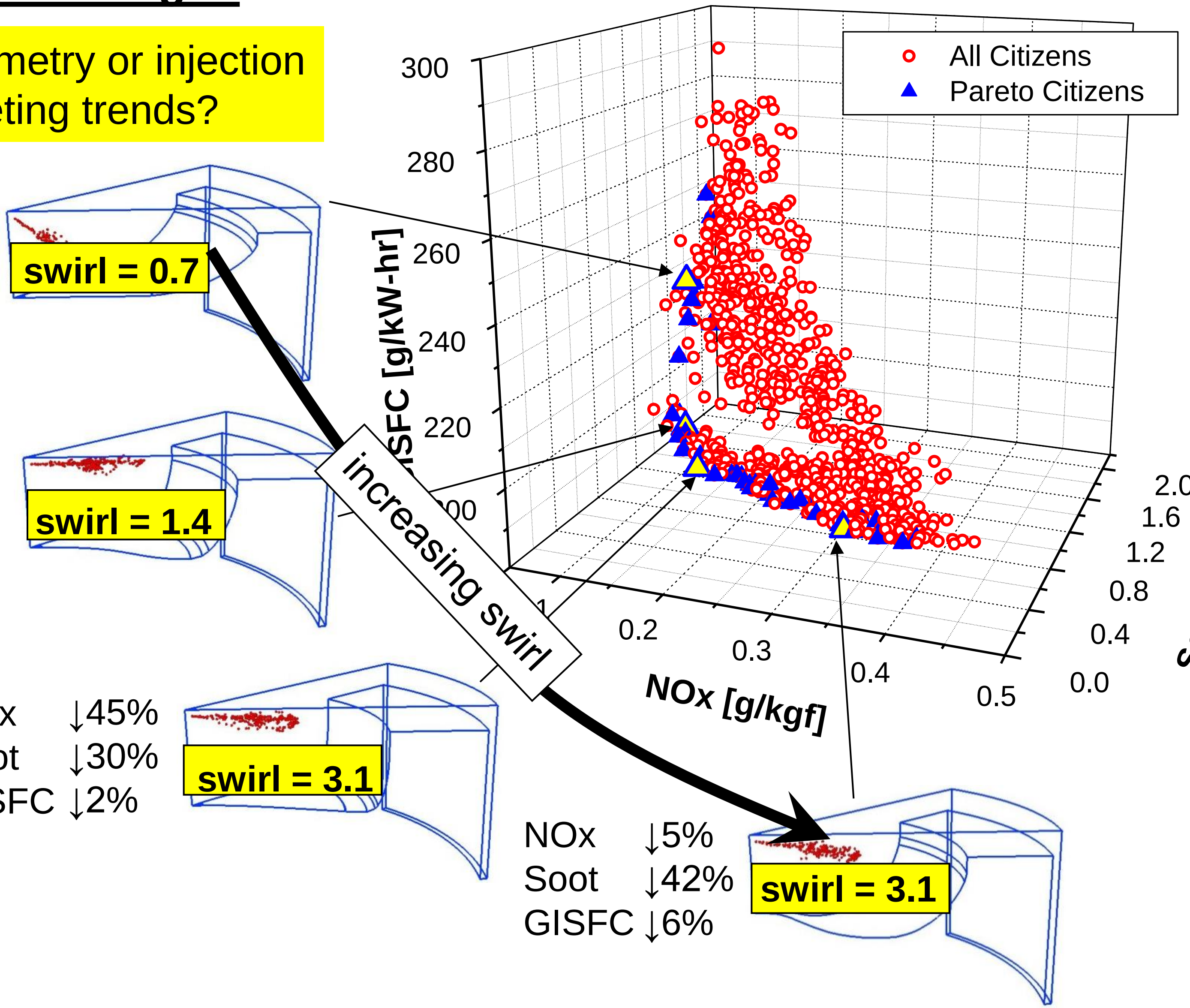
Injector Spray Angle

Swirl Ratio

Genzale, 2007

Pareto front designs

Bowl geometry or injection targeting trends?



NOx ↓68%
Soot ↑77%
GISFC ↑15%

swirl = 0.7

NOx ↓57%
Soot ↑6%
GISFC ↓0%

swirl = 1.4

NOx ↓45%
Soot ↓30%
GISFC ↓2%

swirl = 3.1

NOx ↓5%
Soot ↓42%
GISFC ↓6%

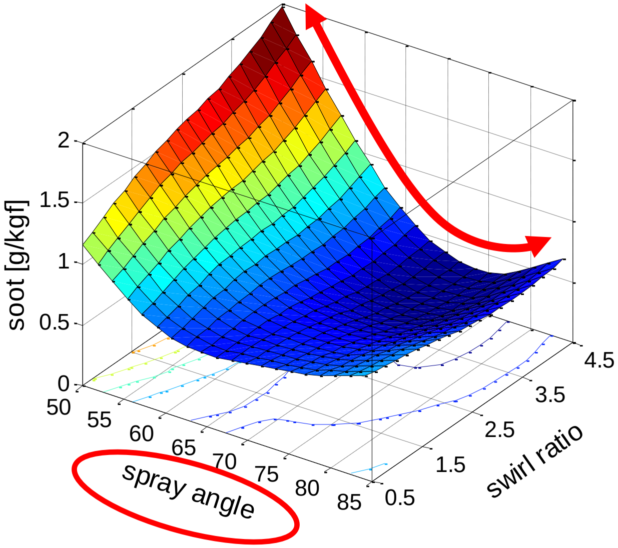
swirl = 3.1

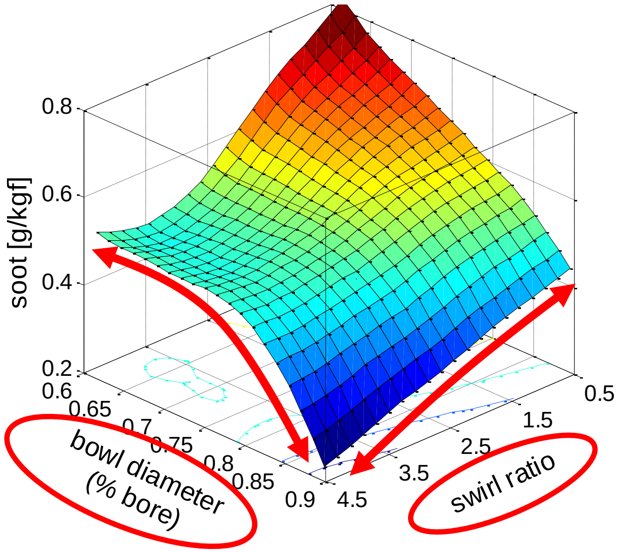
Genzale, 2007

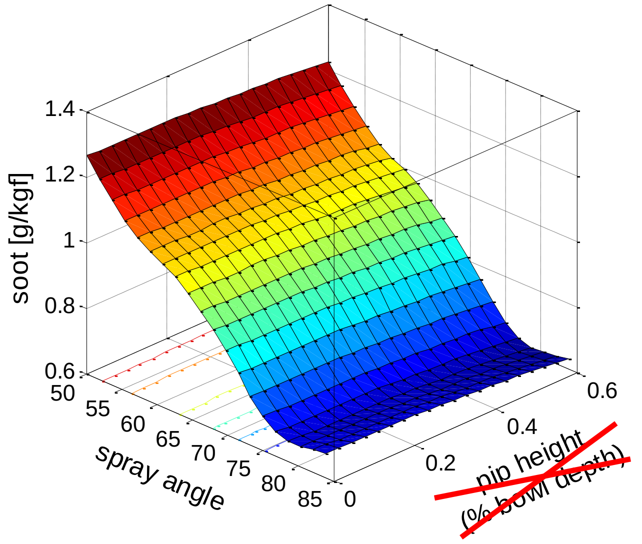
Regression – Identify dominant design parameters

Regression fits performed for each design on the Pareto front

- 3 dominant design parameters identified:
  1. Spray angle
  2. Swirl ratio
  3. Bowl diameter

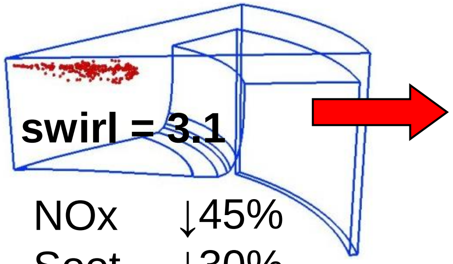




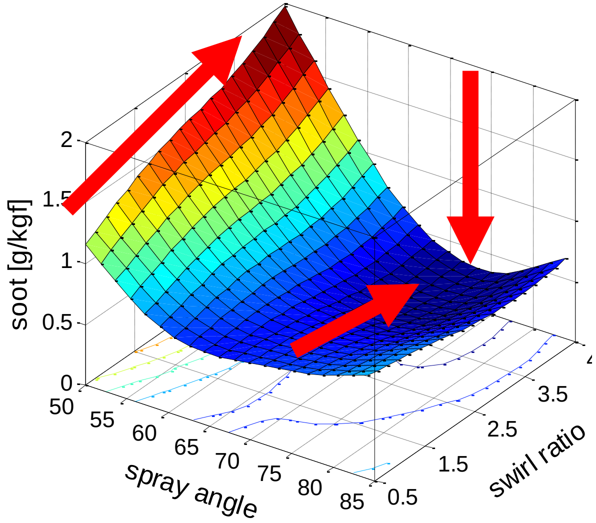


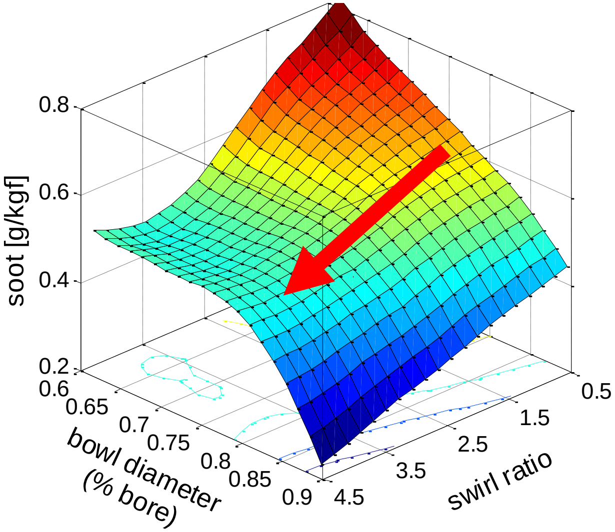
Genzale, 2007

Regression – Understand Parameter Effects



NOx ↓45%
Soot ↓30%
GISFC ↓2%





Response Surface Observations:

An optimal spray angle is predicted.

Increased swirl ratio is predicted to enhance soot reduction near the optimal spray angle.

Increases soot emissions at narrow spray angles.

Increased swirl ratio is predicted to decrease soot at all bowl diameters.

Klingbeil, 2003

Optimization of LTC - low temperature combustion

Increased interest in advanced combustion regimes

RCCI, HCCI, PCCI, MK - offer simultaneous reduction of NOx and soot

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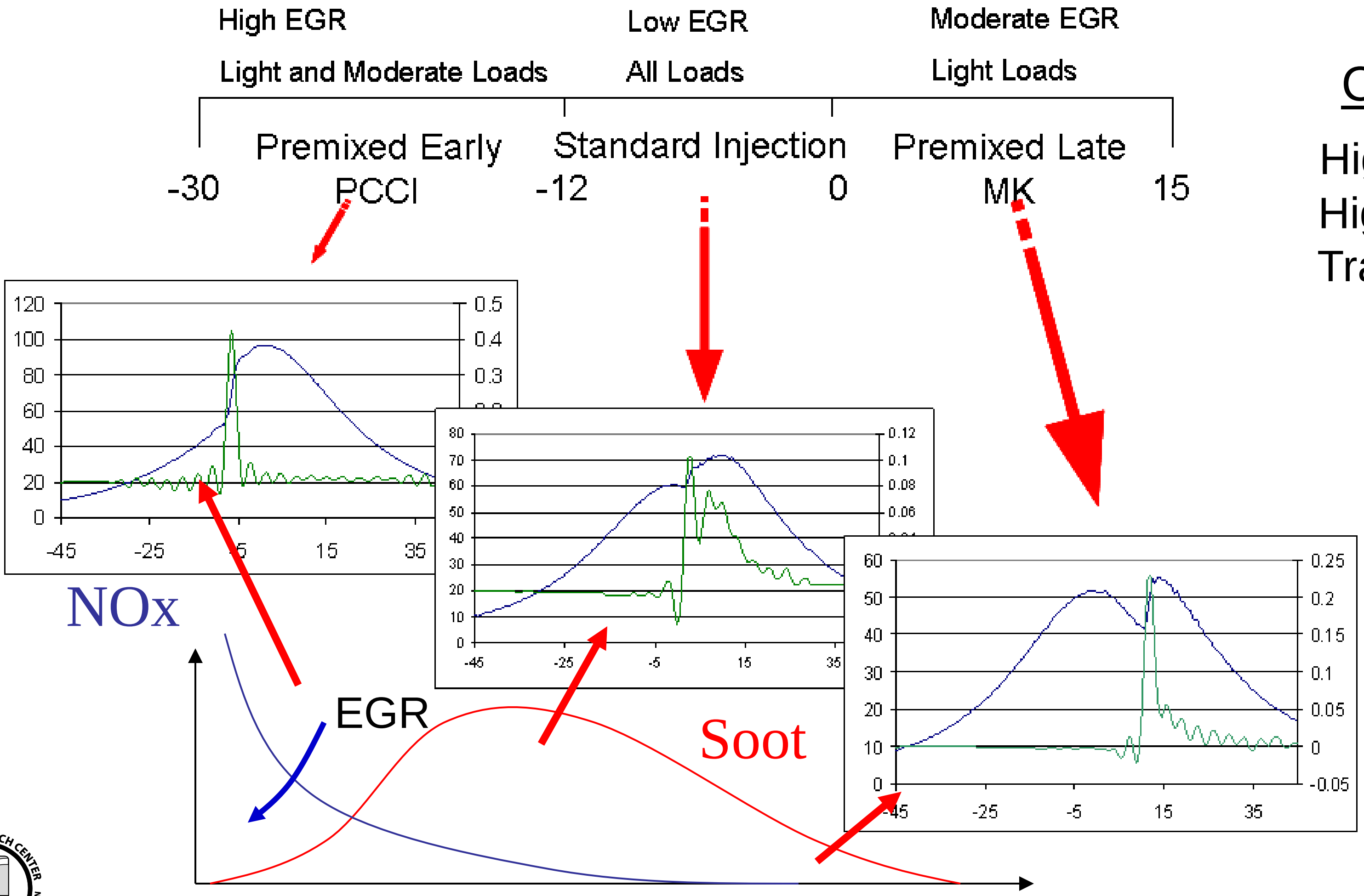


High EGR
Light and Moderate Loads

Low EGR
All Loads

Moderate EGR
Light Loads

Premixed Early
PCCI

Standard Injection

Premixed Late
MK

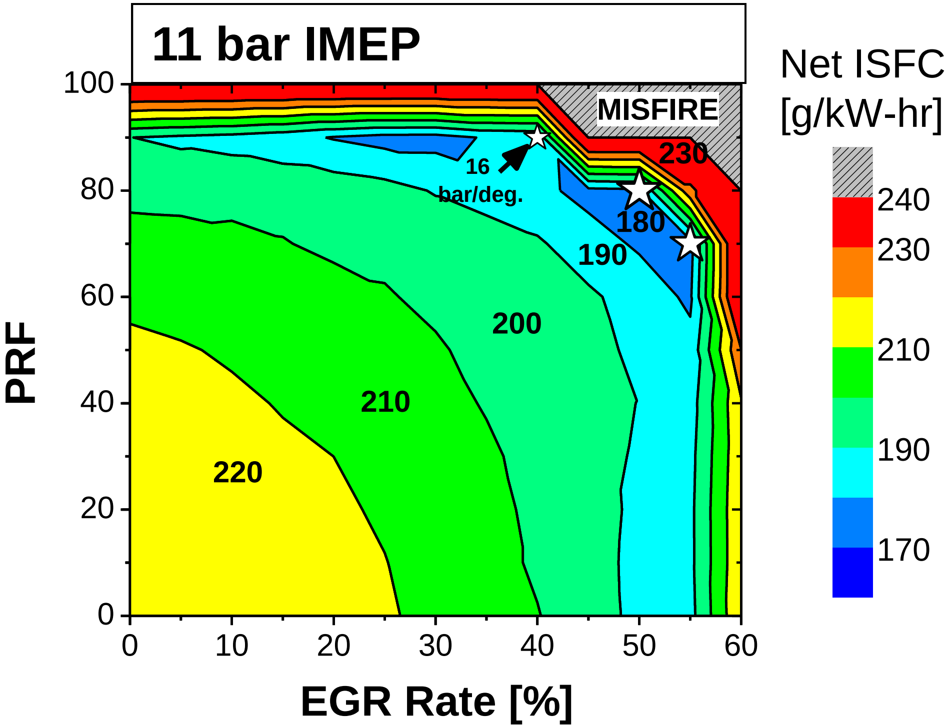
Challenges

High CO, HC
High loads
Transients

Kokjohn, 2009

Combustion optimization - fuel and EGR selection

- HCCI simulations used to choose optimal EGR rate and PRF (isooctane/n-heptane) blend
  - At 6, 9, and 11 bar IMEP
  - 1300 rev/min
- As load is increased the minimum ISFC **cannot** be achieved with either neat diesel fuel of neat gasoline
- Predicted contours are in good agreement with HCCI experiments



Kokjohn, 2009

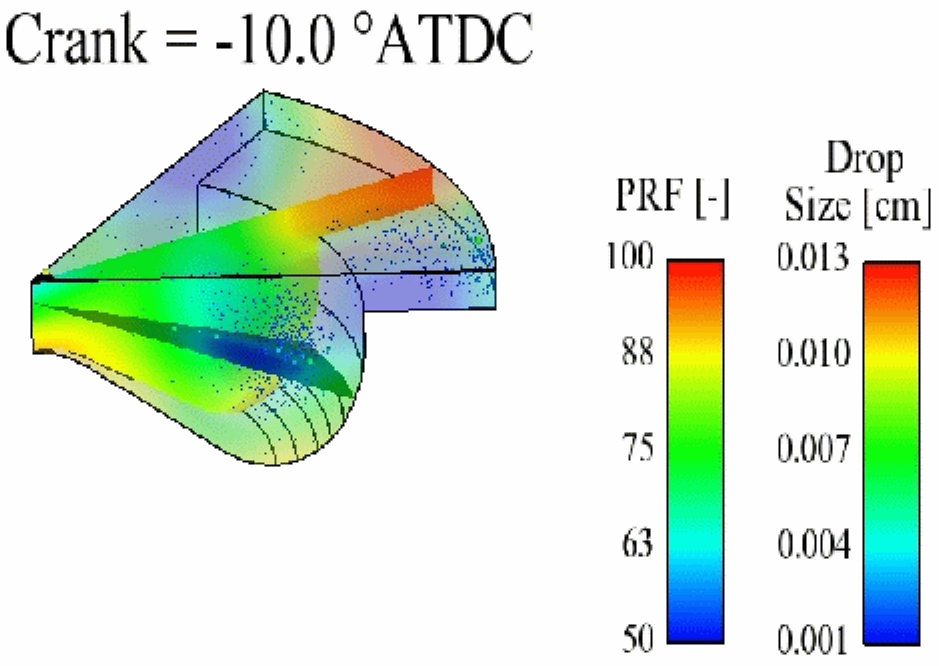
Charge preparation optimization

Premixed and Direct Injected fuel blending

- Desirable to use traditional diesel type injector
  - Large nozzle hole (250 μm)
  - Wide angle (145° included angle)

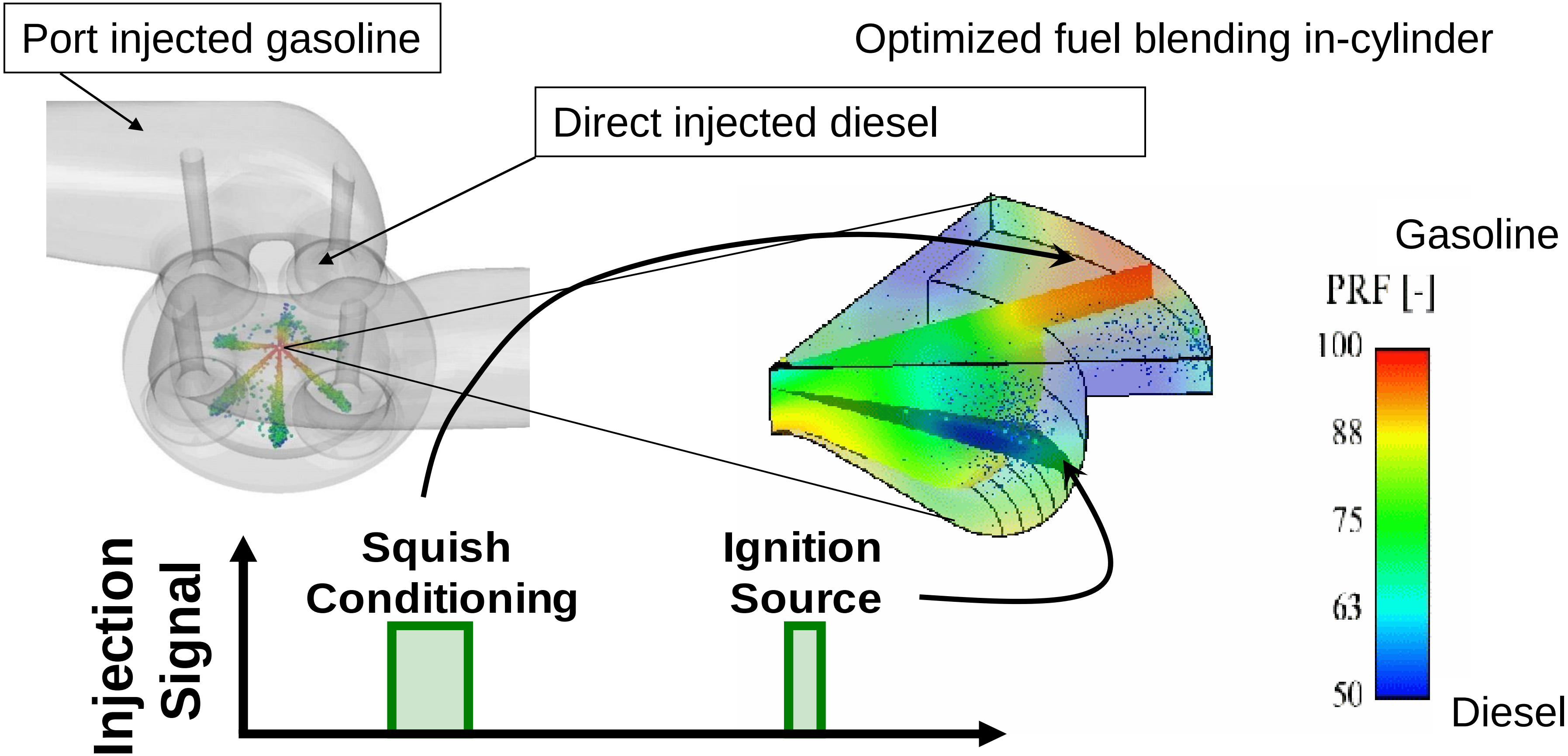
- KIVA + Multi-Objective Genetic Algorithm (MOGA)
- Fuel reactivity and EGR from HCCI investigation (9 bar IMEP)
  - Global PRF = 65
  - EGR rate = 50%
- Five optimization parameters
- Minimize two objectives
  - Wall film amount
  - PRF Inhomogeneity
- Simulations run to 10 °BTDC
- 21 generations with a population size of 24

Inj. 1 Pressure	100 to 1500 bar
Inj. 2 Pressure	100 to 1500 bar
SOI 1	IVC to (SOI2-20) ºATDC
SOI 2	-50 to -30 ºATDC



Kokjohn, 2009

Optimized Reactivity Controlled Compression Ignition (RCCI)



Port injected gasoline

Optimized fuel blending in-cylinder

Direct injected diesel

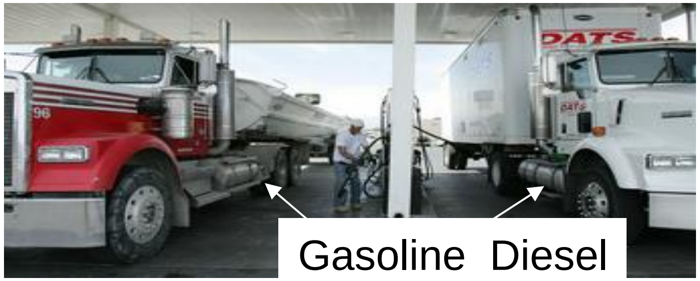
Squish Conditioning

Ignition Source

-80 to -50

-45 to -30

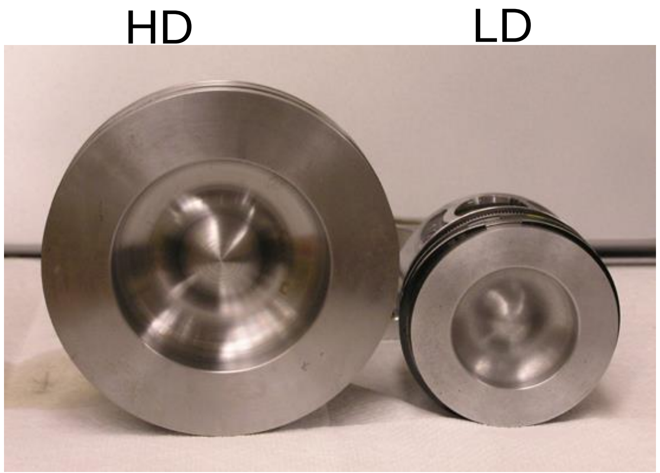
Crank Angle (deg. ATDC)

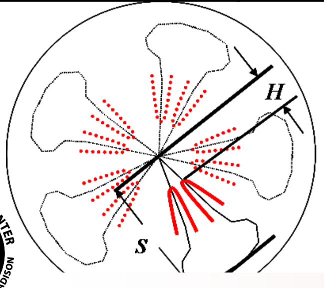


Gasoline Diesel

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



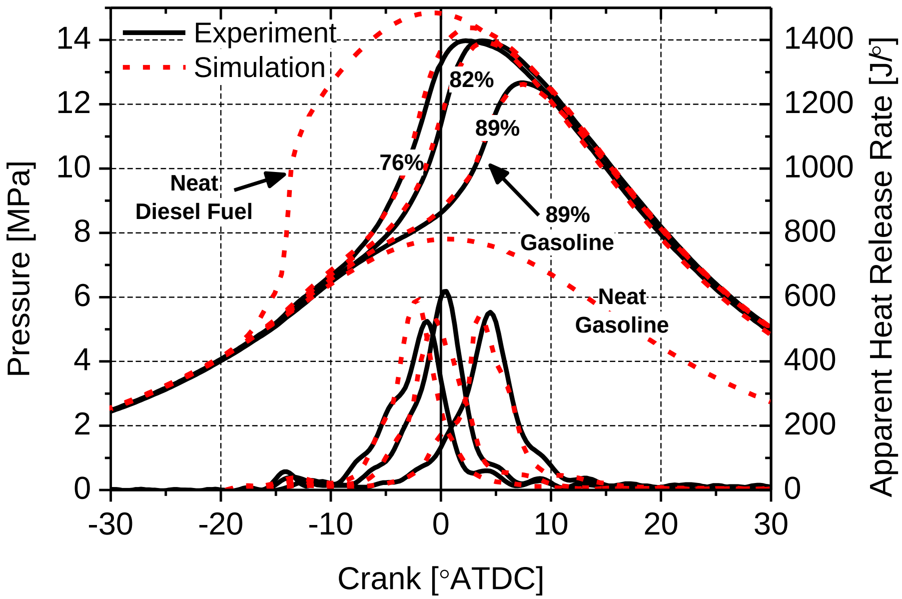


Engine size scaling
Staples, 2009

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 (ºBTDC)/Comp ratio	143/16		

Effect of gasoline percentage



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

Hanson, 2011
Splitter, 2010

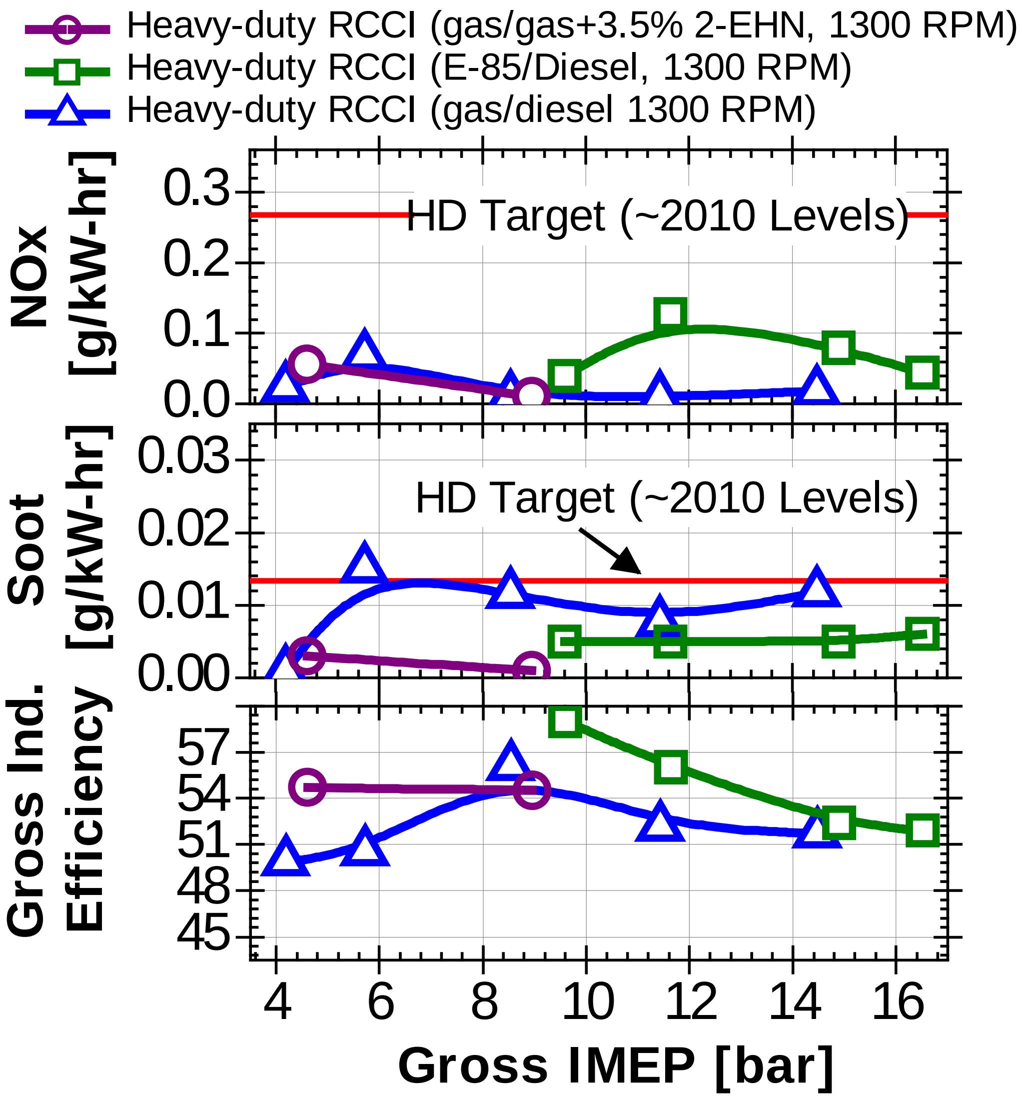
RCCI – high efficiency, low emissions, fuel flexibility

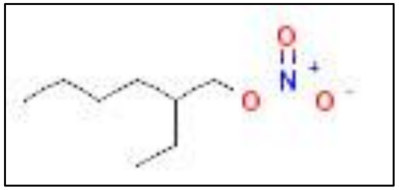
Indicated efficiency of 58±1% achieved with E85/diesel

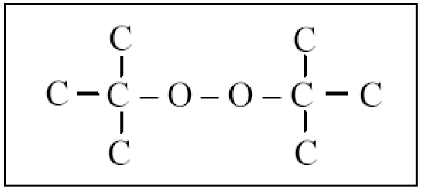
Emissions met in-cylinder, without need for after-treatment

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







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Kokjohn, 2011

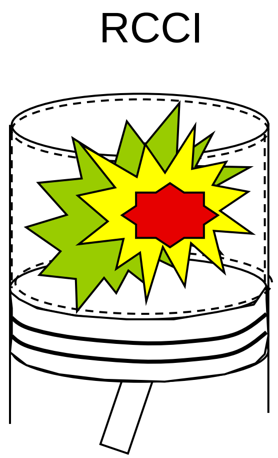
Dual fuel RCCI combustion – controlled HCCI

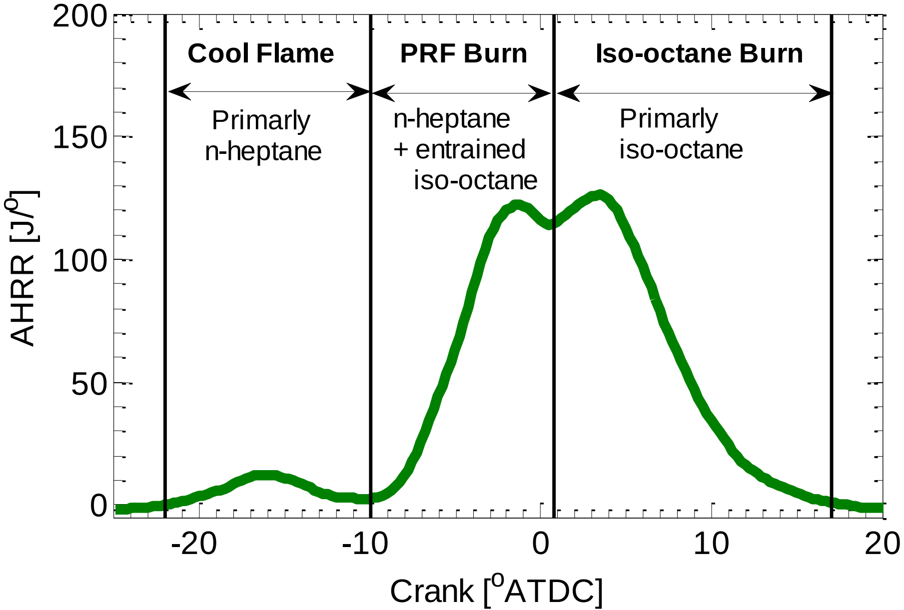
Heat release occurs in 3 stages (SAE 2010-01-0345, 2012-01-0375)

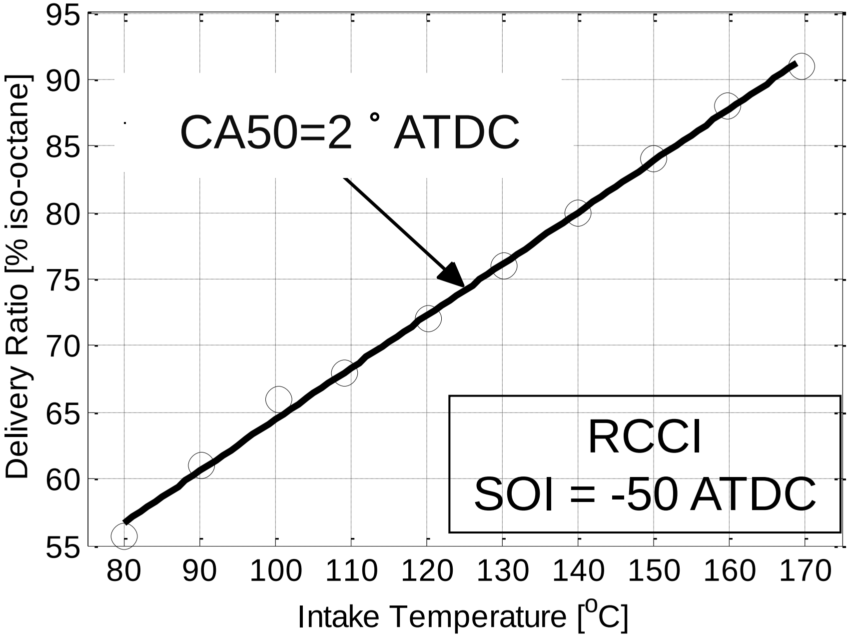
- Cool flame reactions result from diesel (n-heptane) injection
- First energy release occurs where both fuels are mixed
- Final energy release occurs where lower reactivity fuel is located

Changing fuel ratios changes relative magnitudes of stages

Fueling ratio provides “next cycle” CA50 transient control

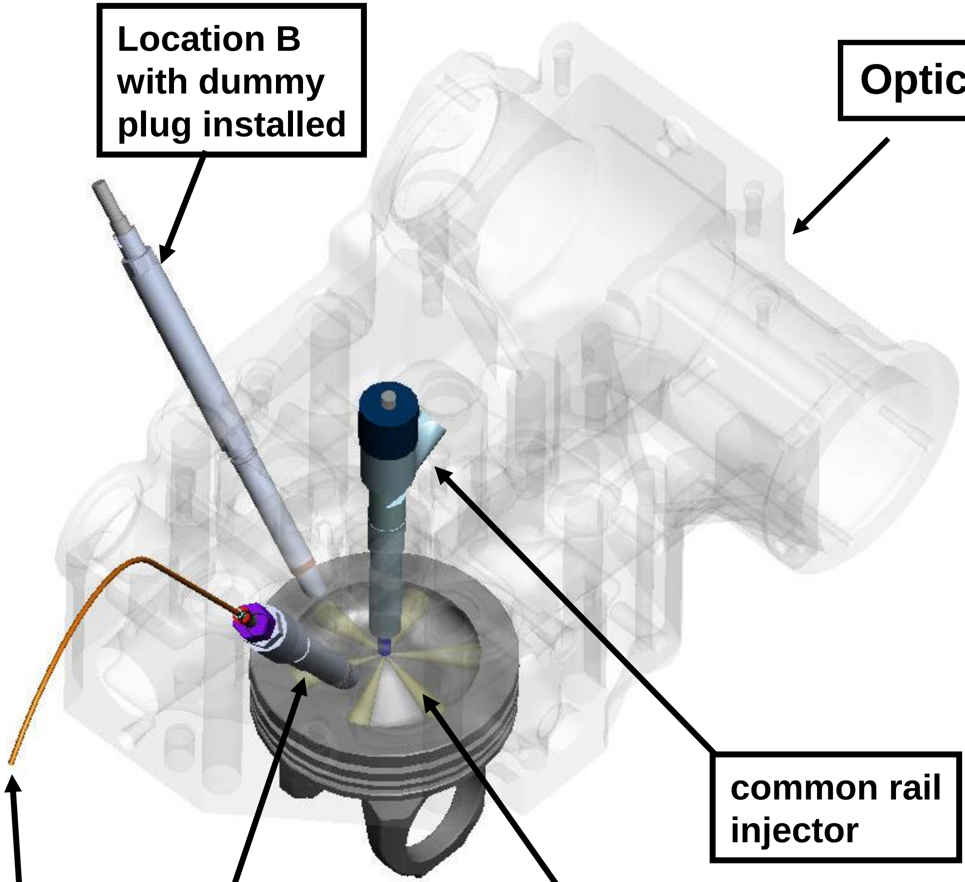






Splitter, 2010

Understanding RCCI combustion



Location B with dummy plug installed

Optical Cylinder Head

common rail injector

Port Fuel Injector

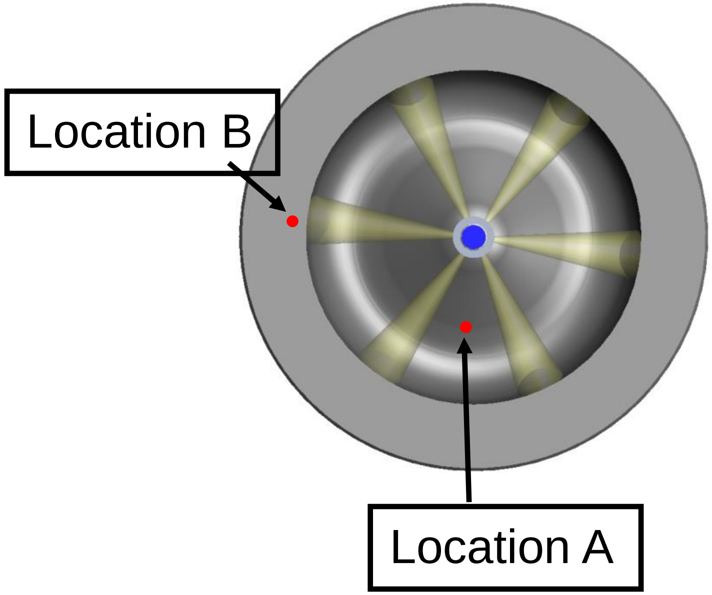
fiber to FTIR

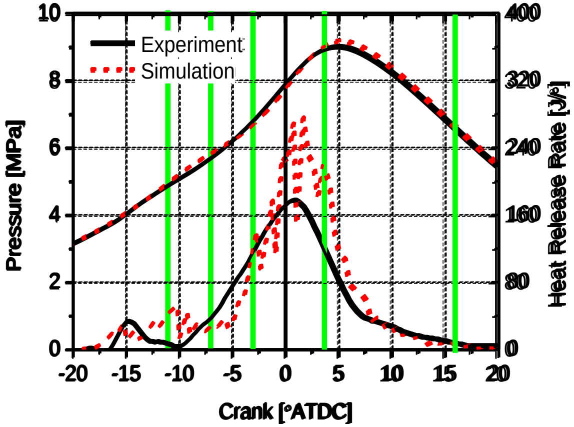
Location A with optics installed

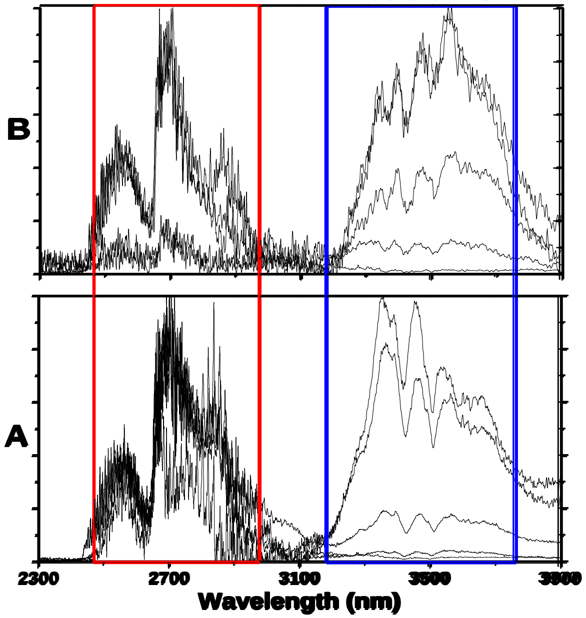
common rail fuel spray

Splitter, 2010

Understanding RCCI combustion







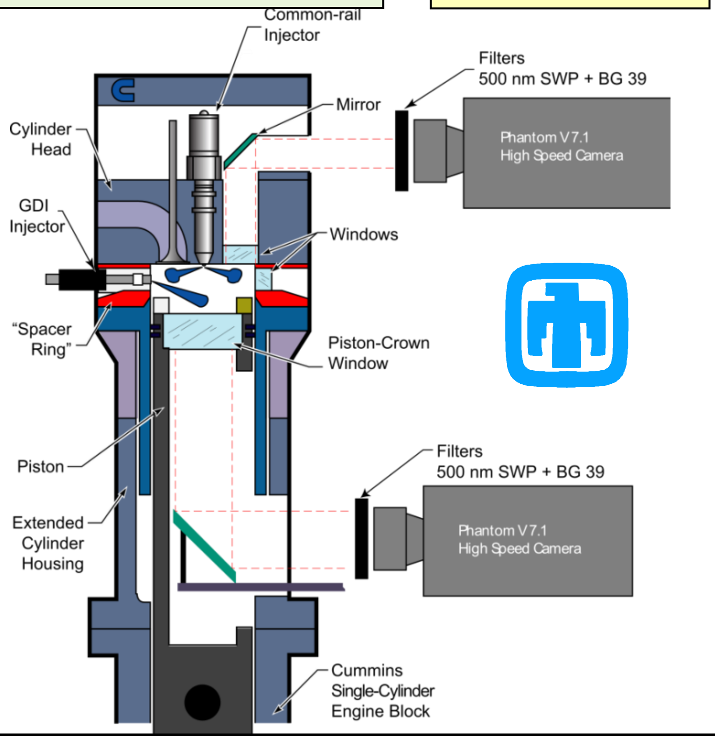
- Experimental in-cylinder FTIR measurements of combustion process at two locations
- Spectra shows different fuel species at locations A and B, a result of the reactivity gradient
- Fuel decomposition and combustion products form at a slower rate at location B, extending combustion duration

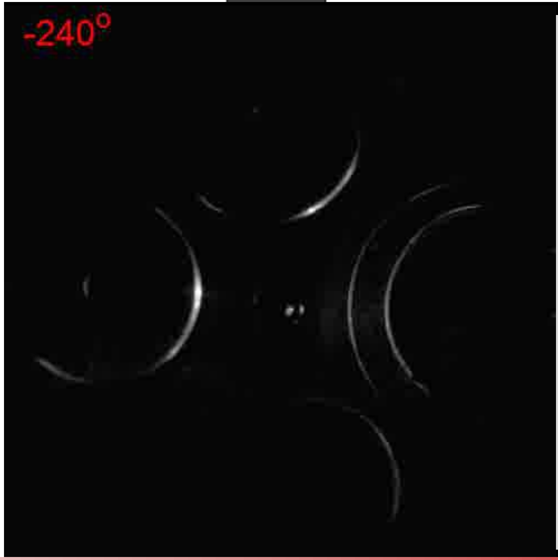
Kokjohn, 2012

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



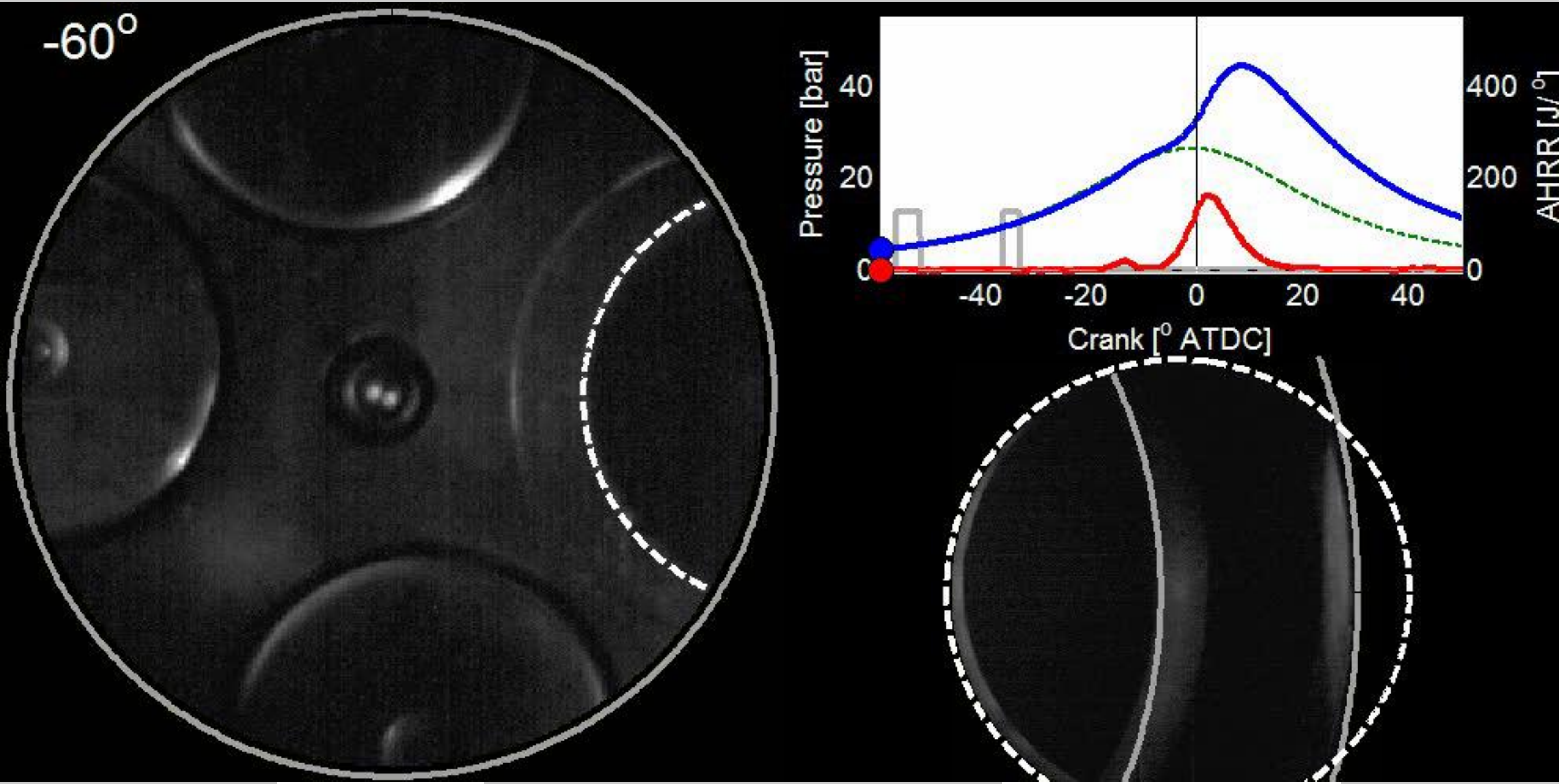


GDI
Iso-octane
100 bar
7x150 micron

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

RCCI combustion luminosity imaging

Load:	4.2 bar IMEP	GDI SOI:	-240°ATDC
Speed:	1200 rpm	CR SOI:	-57°/-37° ATDC
Intake Temperature:	90° C	Equivalence ratio:	0.42
Intake Pressure:	1.1 bar abs.	Iso-octane mass %:	64



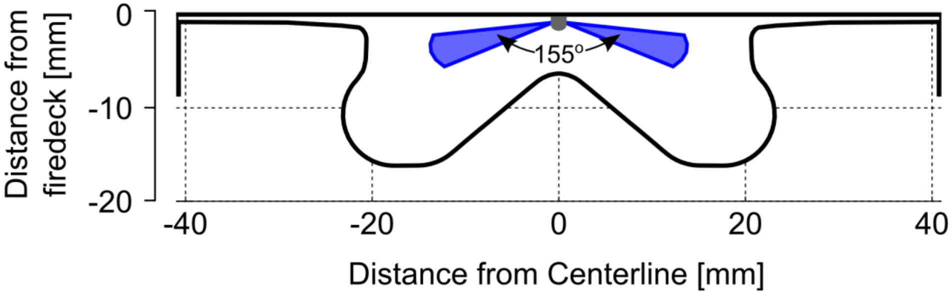
Bowl window

Squish (upper) window

Light-duty drive-cycle performance

- Compare conventional diesel combustion (CDC) and Reactivity Controlled Compression Ignition (RCCI) combustion
- Compare at same operating conditions (CR, boost, IMT, swirl..)
- ERC KIVA-Chemkin Code
  - Reduced primary reference fuel used to model diesel and gasoline kinetics
  - Suite of improved ERC spray models

Combustion Chamber Geometry



Engine specifications

Base engine type	GM 1.9 L
Bore (mm)	82
Stroke (mm)	90.4
Connecting rod length (mm)	145.5
Squish height (mm)	0.617
Displacement (L)	0.4774
Compression ratio	16.7:1
Swirl ratio	1.5 to 3.2
IVC (°ATDC)	-132°
EVO (°ATDC)	112°

Diesel fuel injector specifications

Type	Bosch common rail
Actuation type	Solenoid
Included angle	155°
Number of holes	7
Hole size (μm)	141

Comparison between RCCI and conventional diesel

Five operating points of Ad-hoc fuels working group

Tier 2 bin 5 NOx targets from

Cooper, SAE 2006-01-1145

(assumes 3500lb Passenger Car)

Evaluate NOx / fuel efficiency tradeoff using SCR for CDC

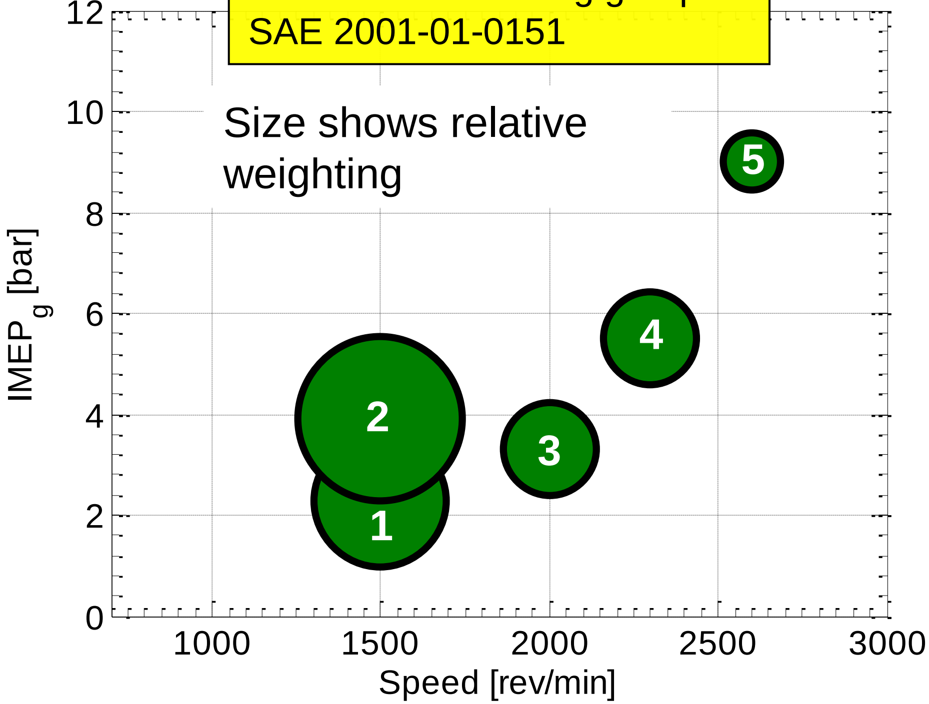
Assumptions

- Diesel exhaust fluid (DEF) consumption is 1% per g/kW-hr NOx reduction

Johnson, SAE 2011-01-0304

- No penalty for DPF regeneration
- UHC and CO only contribute to reduced work

Ad-hoc fuels working group
SAE 2001-01-0151

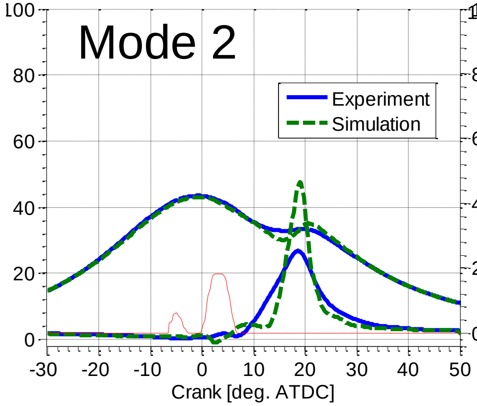


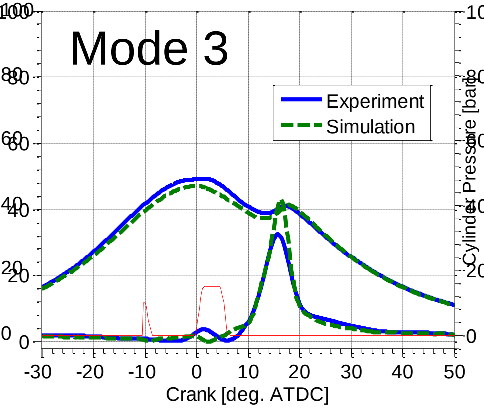
Mode	Speed (rpm)	IMEP (bar)	CDC Baseline NOx (g/kgf) *	NOx Target (g/kgf)
1	1500	2	1.3	0.2
2	1500	3.9	0.9	0.4
3	2000	3.3	1.1	0.3
4	2300	5.5	8.4	0.6
5	2600	9	17.2	1.2

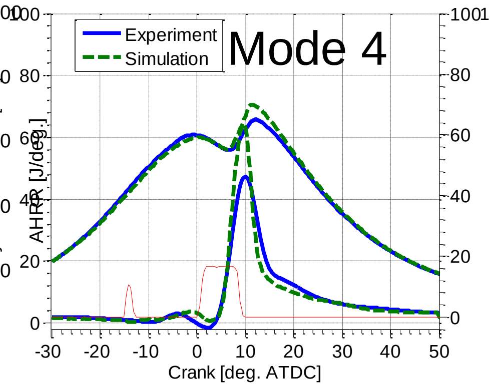
* Baseline CDC Euro 4: Hanson, SAE 2012-01-0380

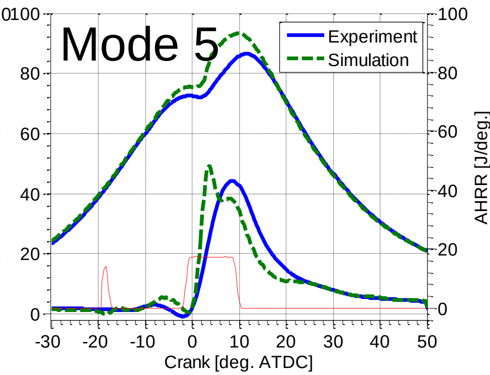
Euro 4 operating conditions - conventional diesel

Model validation	CDC Operating Conditions *				
Mode	1	2	3	4	5
IMEPg (bar)	2.3	3.9	3.3	5.5	9
Speed (rev/min)	1500	1500	2000	2300	2600
Total Fuel (mg/inj.)	5.6	9.5	8	13.3	20.9
Intake Temp. (deg. C)	60	60	70	67	64
Intake Press. (bar abs.)	1	1	1	1.3	1.6
EGR Rate (%)	47	38	42	25	15
CR Inj. Pressure (bar)	330	400	500	780	1100
Pilot SOI advance (°CA)	7	7	11	15	18
Main SOI (° ATDC) (actual)	-0.9	0	0.1	0.5	-1.8
Percent of DI fuel in Pilot (%)	20	15	15	10	10



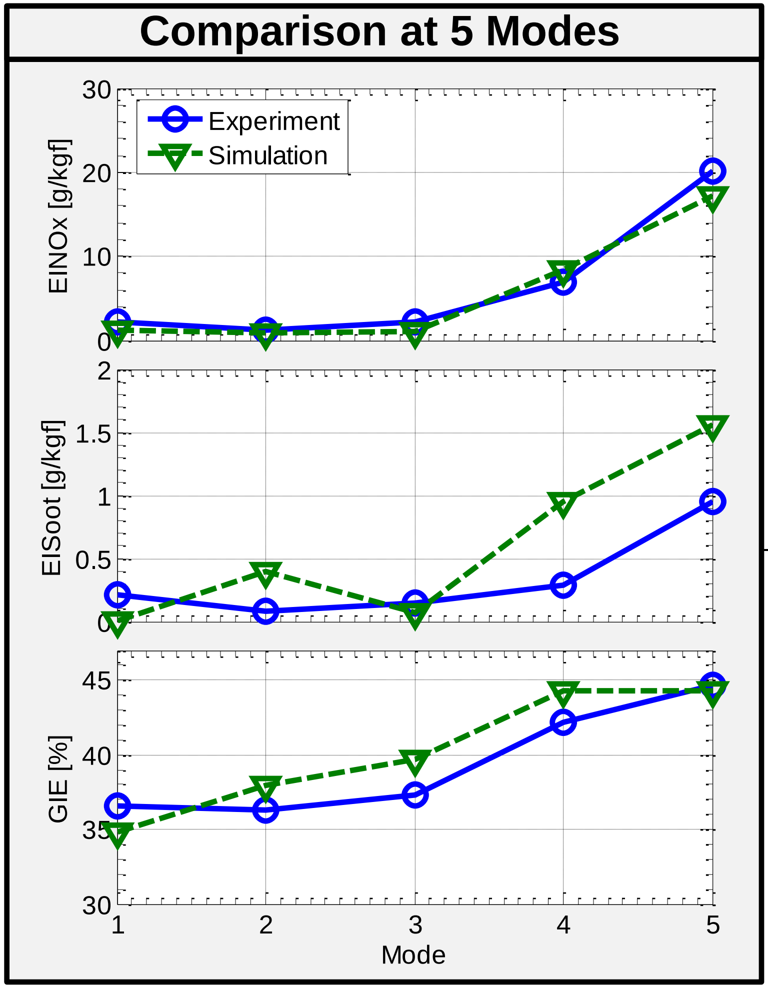






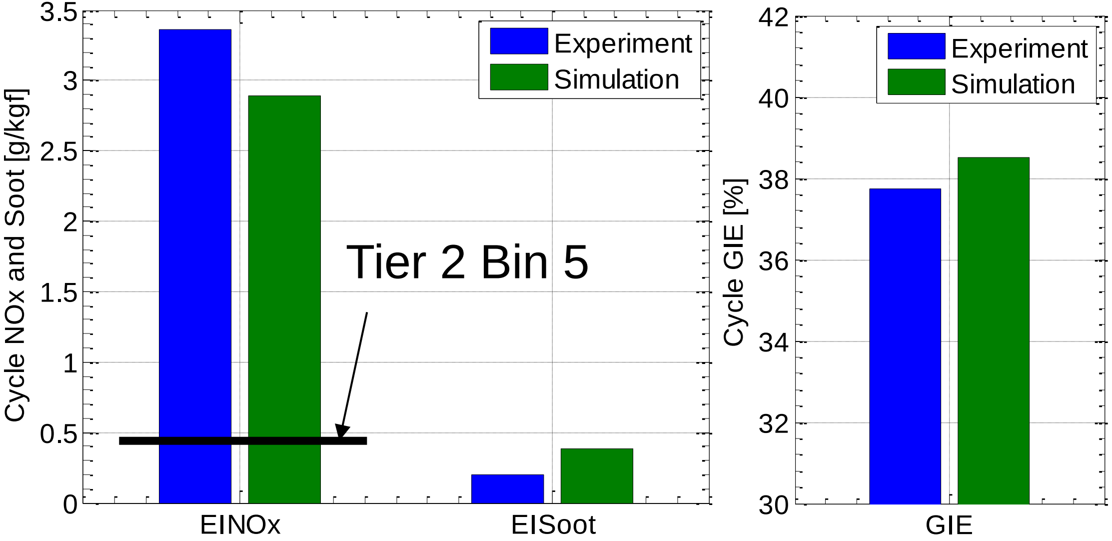
* Baseline CDC Euro 4: Hanson, SAE 2012-01-0380

Model validation (Euro 4)

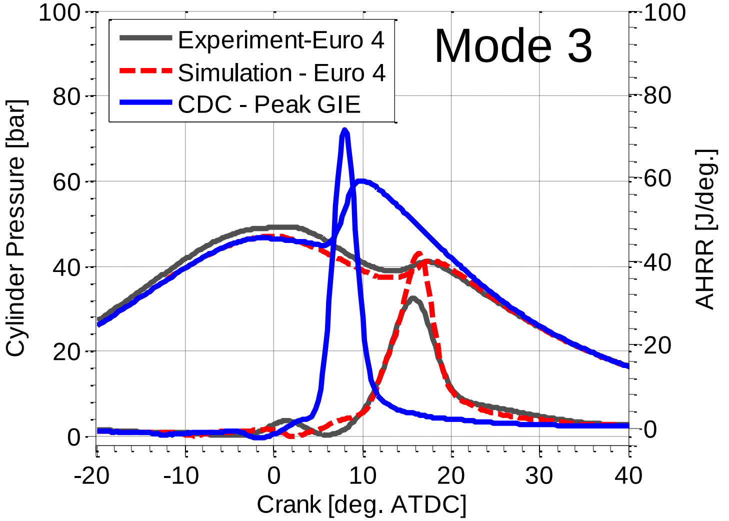

Comparison at 5 Modes

Weighted average: $$E_{cycle} = \frac{\sum_{imode=1}^{5} E_{imode} Weight_{imode}}{\sum_{imode=1}^{5} Weight_{imode}}$$

Cycle average emissions and performance



Optimized CDC with SCR for Tier 2 Bin 5



CDC optimized GIE has higher allowable PPRR (advanced SOI) than Euro 4 calibration

Kokjohn, 2013

Comparison between RCCI and conventional diesel

"CDC Peak GIE" point shown for reference (does not meet NOx target)

CDC and RCCI efficiency sensitive to selected value of peak PRR

- Maximum allowable PRR of CDC points set at 1.5 times higher than for RCCI

	CDC	**RCCI**	**CDC**	**RCCI**	**CDC**	**RCCI**	**CDC**	**RCCI**	**CDC**	**RCCI**
Mode	1		2		3		4		5	
IMEPg (bar)	2.3		3.9		3.3		5.5		9	
Speed (rev/min)	1500		1500		2000		2300		2600	
Total Fuel (mg/inj.)	5.6		9.5		8		13.3		20.9	
Intake Temp. (deg. C)	60		60		70		67		64	
Intake Press. (bar abs.)	1		1		1		1.3		1.6	
EGR Rate (%)	47	61	38	0	42	0	25	0	15	36
Premixed Gasoline (%)	0	0	0	65	0	48	0	79	0	90
CR Inj. Pressure (bar)	330	500	400	500	500	500	780	500	1100	500
Pilot SOI advance (°CA)	7	16	7	21	11	21	15	N/A	18	21
Main SOI (° ATDC) Baseline	-0.9	-17	0	-37	0.1	-37	0.5	-60	-1.8	-37
Main SOI (° ATDC) Peak GIE	-4.6	N/A	-1.3	N/A	-4.1	N/A	-3.6	N/A	-8	N/A
Main SOI (° ATDC) Bin 5 SCR	-4.6	N/A	-1.3	N/A	-4.1	N/A	**-2**	N/A	**-6.3**	N/A
Percent of DI fuel in Pilot (%)	20	42	15	60	15	60	10	0	10	60
DEF (%)	0.6	0	0.4	0	0.5	0	2.1	0	4.9	0

Kokjohn, 2013

RCCI vs. CDC + SCR

CDC (with SCR)

Main injection timing swept

DEF consumption 1% per 1 g/kW-hr reduction in NOx

$$GIE_{Total} = \frac{Work_{-180\ \text{to}\ 180}}{(m_{DEF} + m_{Fuel}) * LHV_{Fuel}} \times 100$$

Peak efficiency at tradeoff between fuel consumption (SOI timing) and DEF consumption (engine-out NOx)

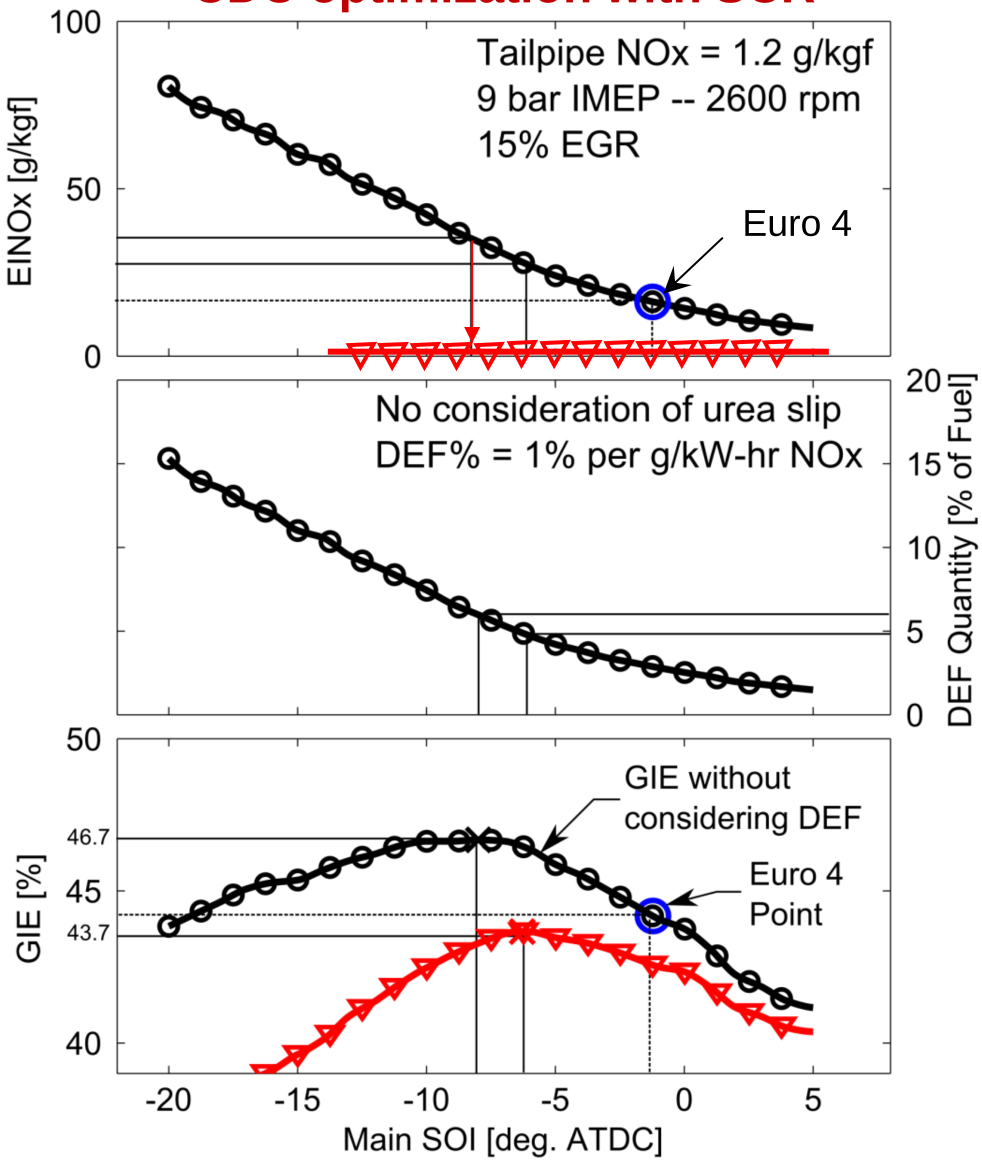
RCCI (No SCR needed)

Gasoline amount controls CA50 to meet NOx/PRR constraints

Mode 1 uses diesel LTC (i.e., no gasoline and EGR is added)

Mode 5 has EGR for phasing control

CDC optimization with SCR



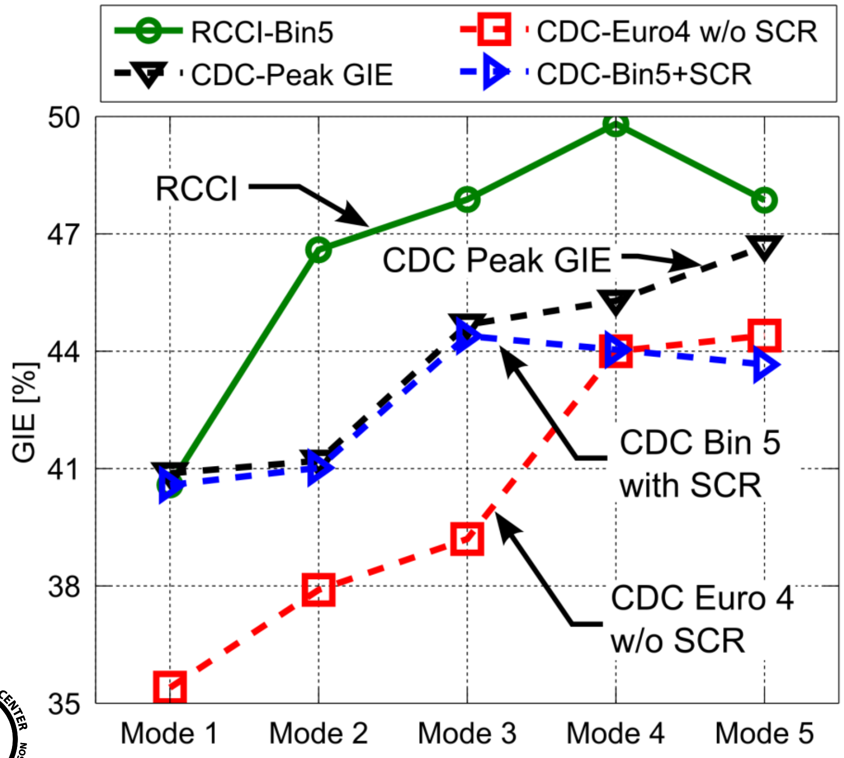
Comparison of efficiency, NOx and PRR

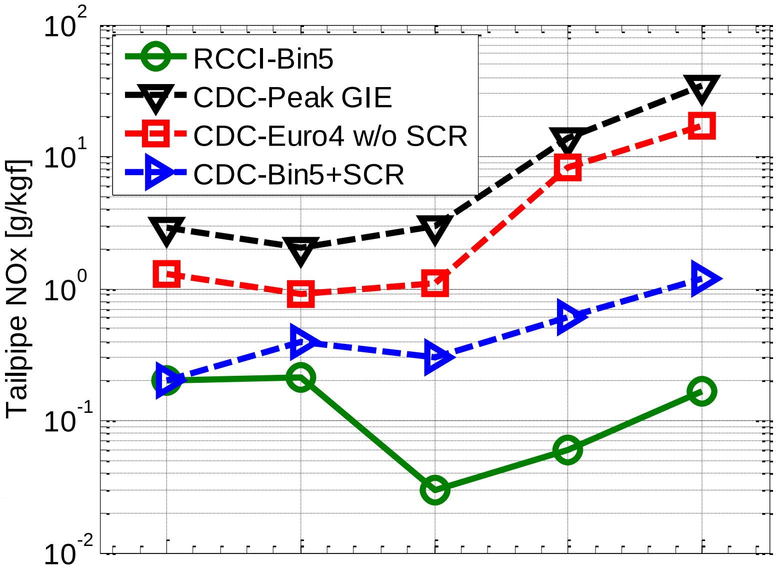
Target NOx at Tier 2 Bin 5

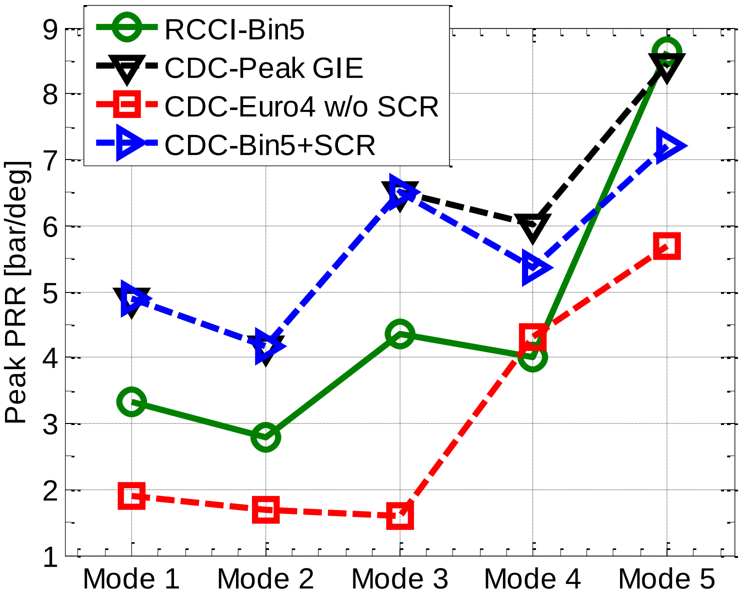
RCCI meets NOx targets without DEF

DEF NOx after-treatment has small efficiency penalty at light-load (2 to 4 bar IMEP) and moderate EGR (~40%)

DEF penalty is larger above 5 bar IMEP where EGR is below 40%



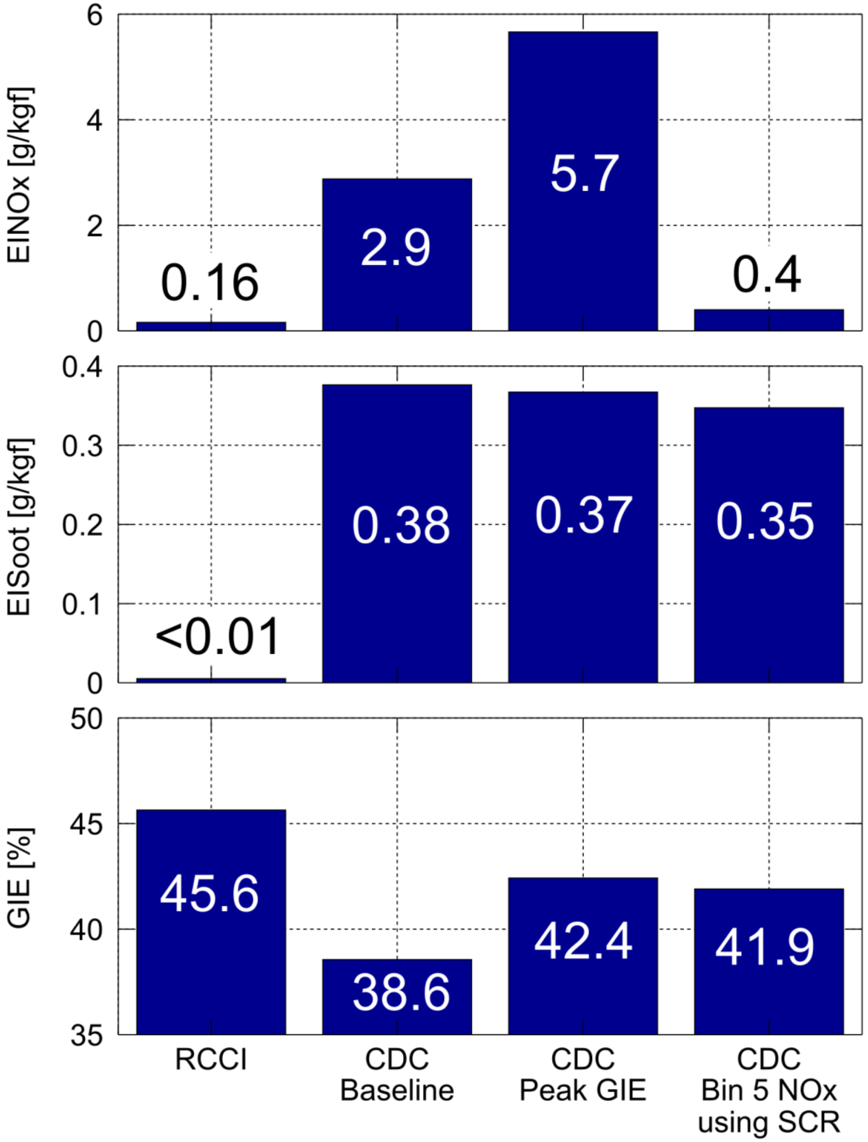




Cycle averaged NOx, Soot and GIE

- RCCI and CDC compared at baseline and Tier 2 Bin 5 NOx
  - CDC NOx-GIE tradeoff controlled by main injection timing
- RCCI meets NOx targets without after-treatment
- RCCI gives ~8% improvement in fuel consumption over CDC+SCR
- RCCI soot is an order of magnitude lower than CDC+SCR
- RCCI HC is ~5 times higher than CDC+SCR
  - Currently addressing methods to reduce HC emissions
  - Crevice-originated HC emissions

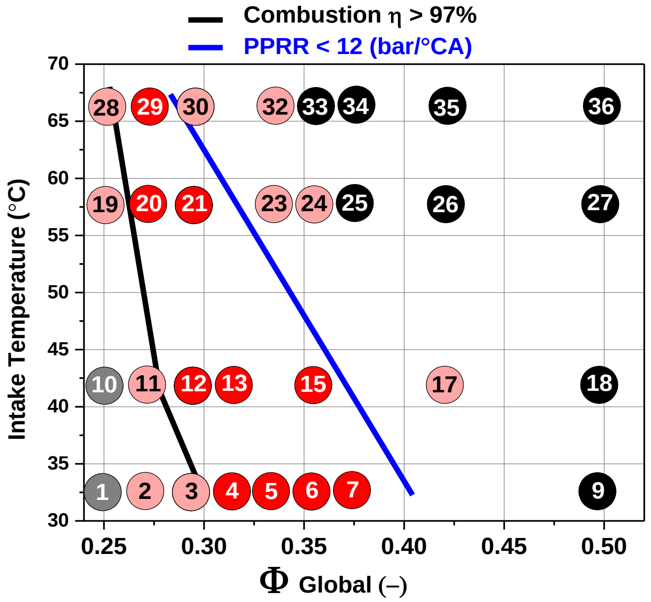
    Splitter, SAE 2012-01-0383
  - Thermal barrier coated piston



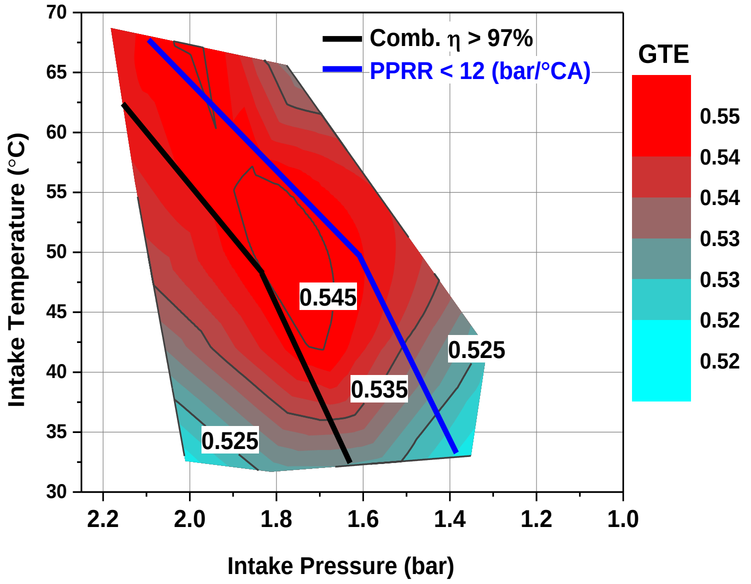
Optimizing RCCI efficiency

Heavy-duty SCOTE engine

IMEPn (bar)	**8.45±.05**
CA50 (°CA ATDC)	**0.5±.5**
Speed (rev/min)	**1300**
Piston Bowl Shape	**Bathtub**
Cr (-)	**14.88:1**
DI Timing (°CA ATDC)	**-60/-35**
DI Bias (%SOI1, % SOI2)	**~60/40**
PFI Timing (°CA ATDC)	**-320**
EGR (%)	**0**
Intake Temperature (°C)	**32-66 (varied)**
Intake Pressure (bar)	**1.31-2.18 (varied)**
Exhaust Pressure (bar)	**Fixed turbo. η**
Overall Turbo η (%)	**~65 (simulated)**
PFI Fraction (-)	**0.49-0.78 (varied)**
DI Fraction (-)	**0.51-0.22 (varied)**

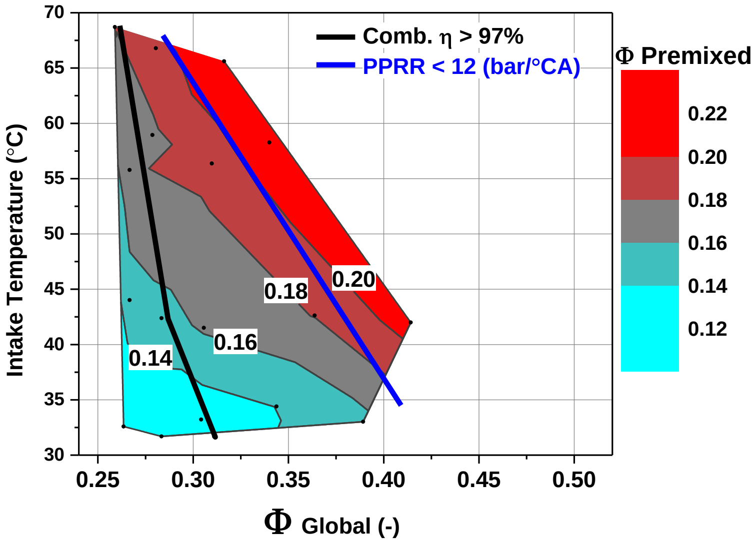


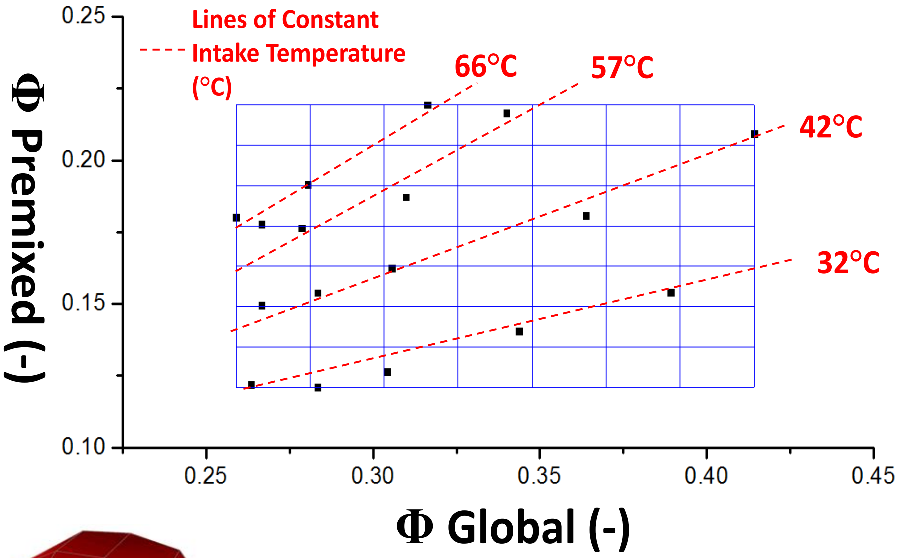
GTE vs. intake pressure & temperature



Splitter, 2014

Premixed vs. global Φ & intake temp

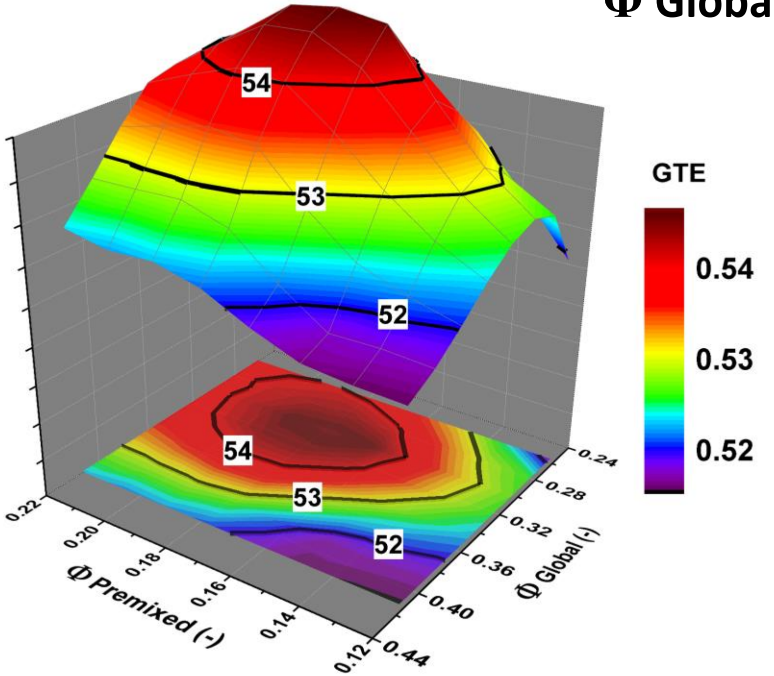




CA50 ~ TDC

Fueling:
DI=3% 2-EHN in 91 PON gas
PFI=E85

Highest GTE occurs at lean conditions with ~63% of charge fully premixed



Limits of dual-fuel RCCI efficiency ?

- Calibrate 0-D code with CR=14.88 experiments
- Use code to determine conditions needed to reach ~ 60% GTE

Results:

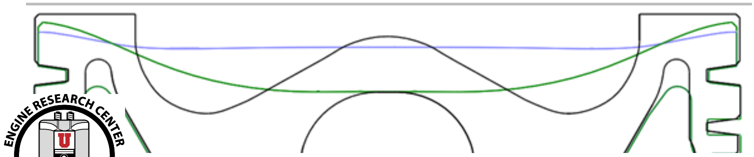
~60% GTE possible with:

High Cr

Lean operation ($\Phi<0.3$)

50% reduction in heat transfer & combustion losses

- Deactivate under-piston oil jet cooling

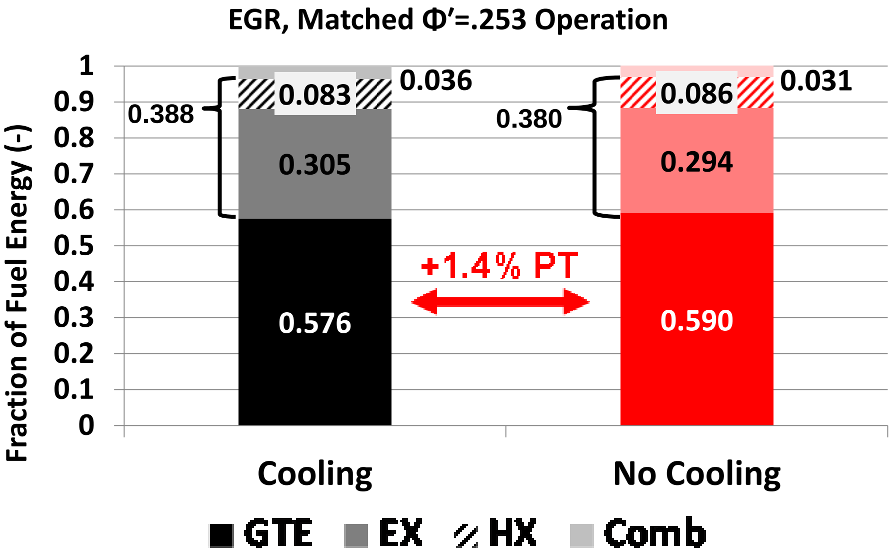


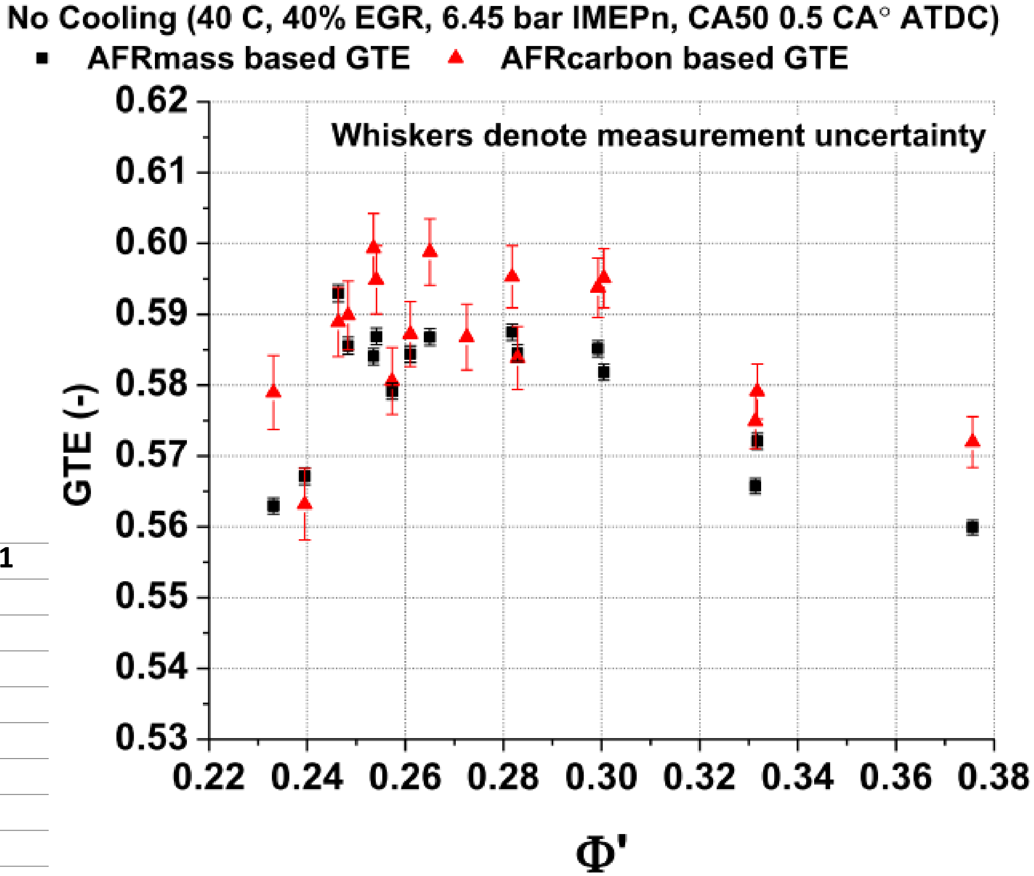
	Exp.	GT POWER
Compression ratio	**14.88**	**14.88**
IMEPn (bar)	**8.00**	**7.86**
Fueling (mg/cyc)	**87.13**	**87.13**
Gross Therm Eff. (%)	**54.3**	**54.5**
Net Therm Eff. (%)	**52.0**	**52.1**
BTE (%)	**45.3**	**45.1**
FMEP (bar)	**1.03**	**1.0**
Convection HX	**N/A**	**0.4**
Comb. Eff. (%)	**98**	**98**
Intake Pressure (bar)	**1.5**	**1.5**
Exhaust Pressure (bar)	**1.625**	**1.625**
Turbo eff. (air filter + DOC)	**67.5**	**62.3**

Splitter, 2013

GTE with / without oil jet cooling

- Largest advantage in GTE observed at lean conditions
- High GTE Realized
  - Close to 60%





Ultra-high efficiency dual-fuel RCCI combustion

	GTE (%)	IMEPg (bar)	NTE (%)	IMEPn (bar)
EXP (pt. 83)	**59.1**	**6.82**	**55.0**	**6.27**
GT Power HX =0.2	**58.8**	**6.79**	**54.8**	**6.25**
GT Power HX =0.4	**56.7**	**6.55**	**52.8**	**6.02**

High efficiency demonstrated!

Simulation heat transfer tuned to match data

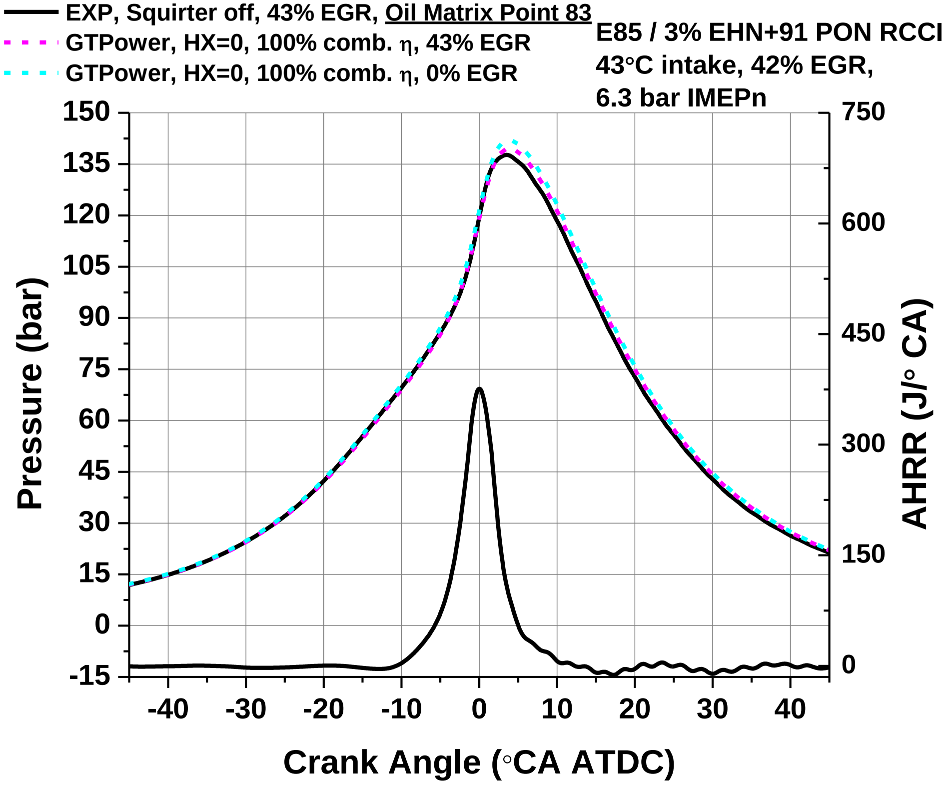
14.88:1 required HX = 0.4

18.7:1 required HX = 0.3

(Pancake ~1.2 less surface area)

18.7:1 w/o oil cooling HX = 0.2

	GTE (%)	IMEPg (bar)	NTE (%)	IMEPn (bar)
Experiment	59.1	6.82	55.0	6.27
Model, HX =0 100% comb. η	62.4	7.12	58.5	6.85
Model, HX =0 100% comb.η, 0% EGR	63.4	7.23	61.0	6.95



94% of maximum theoretical cycle efficiency achieved !

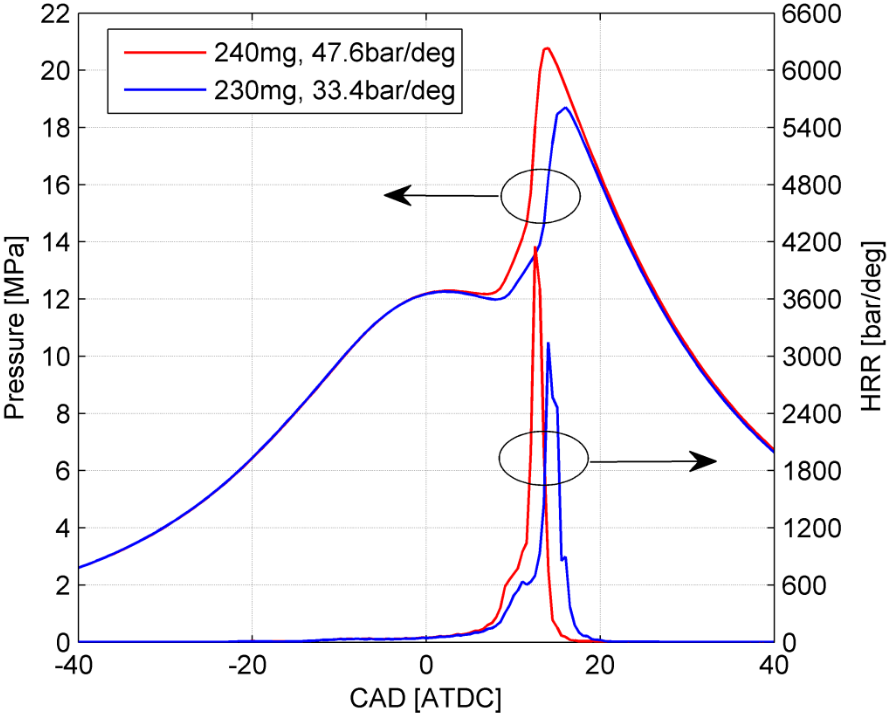
Splitter, "RCCI Engine Operation Towards 60% Thermal Efficiency", SAE 2013-01-0279

Extending RCCI load range

High load RCCI attempt with gasoline/diesel leads to HCCI

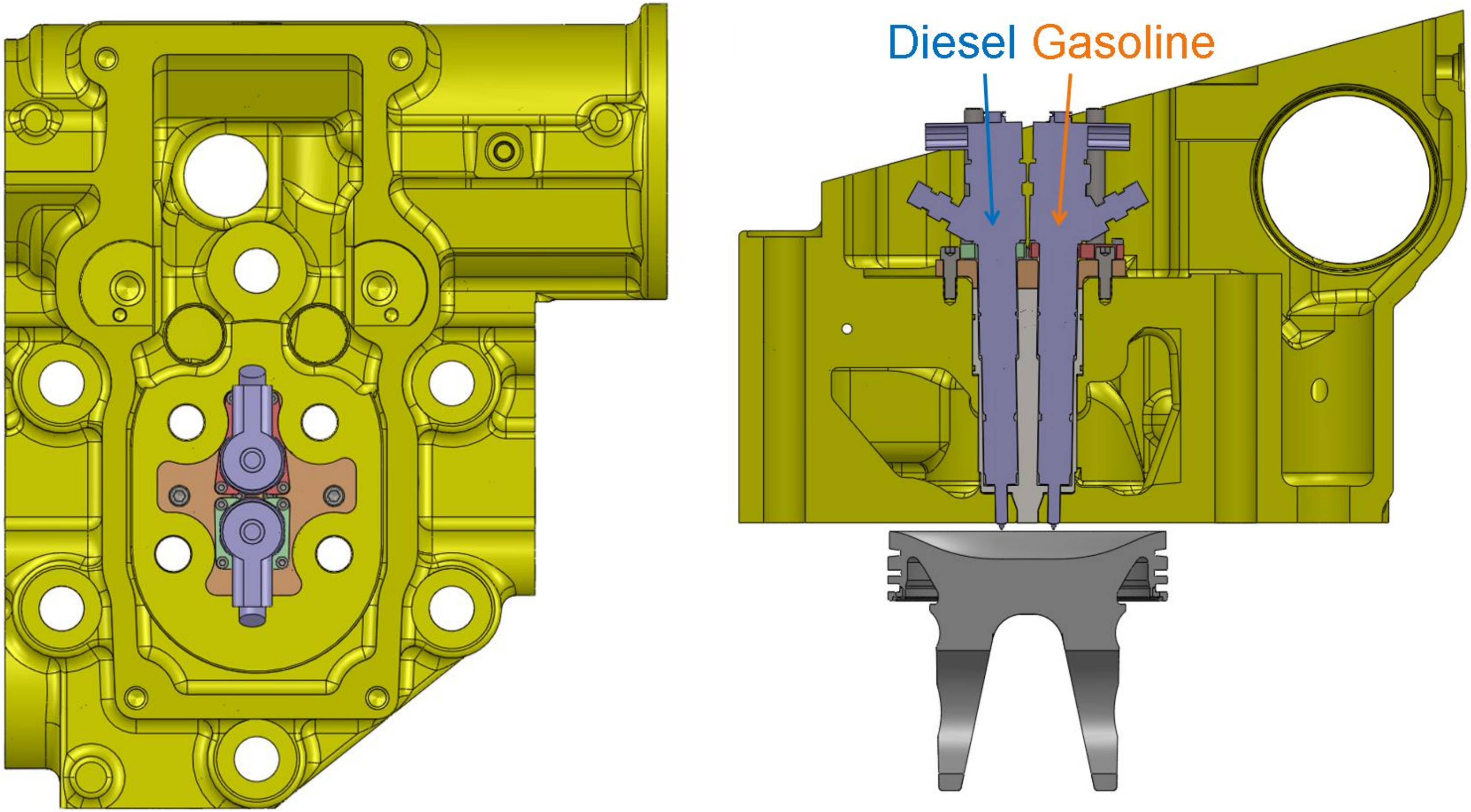
Conventional RCCI: Low reactivity fuel (i.e., gasoline or iso-octane) is port-injected, and high reactivity fuel (i.e., diesel or n-heptane) is direct-injected.

- 21bar IMEP requires ~245mg of fuel.
- 3.42bar, 90°C, 46%EGR @ IVC, 1800 rev/min leads to HCCI combustion when iso-octane is port-injected.
- Use two direct injectors to provide more flexibility



Extending RCCI load range

Independent Stratification of Reactivity and Equivalence Ratio with Dual Direct Injection

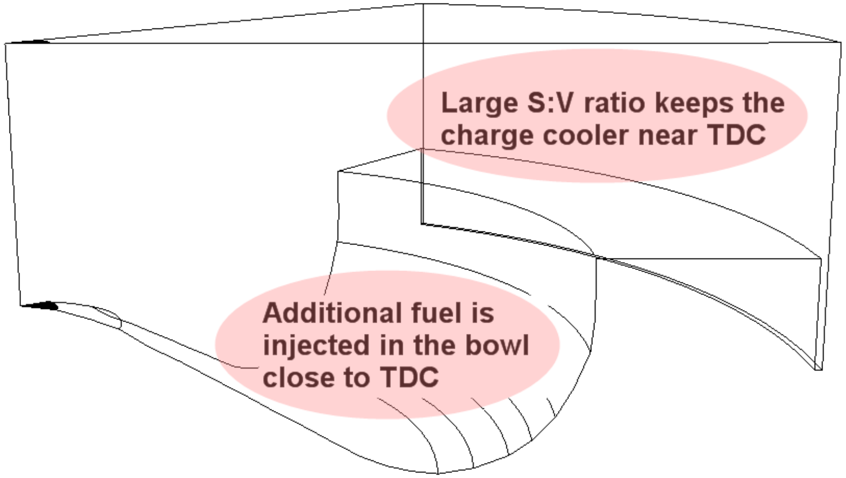


Extending RCCI load range

Allows utilization of piston geometry

- IVC condition: 3.42bar, 90°C, 46%EGR
- Direct injection of iso-octane can place fuel in different locations at different timings.
- The stock piston geometry creates 2 combustion zones.
  - Squish with high surface:volume ratio
  - Bowl with low S:V ratio

- If fuel is placed in the squish region, its reaction rate can be controlled by heat transfer to the walls.



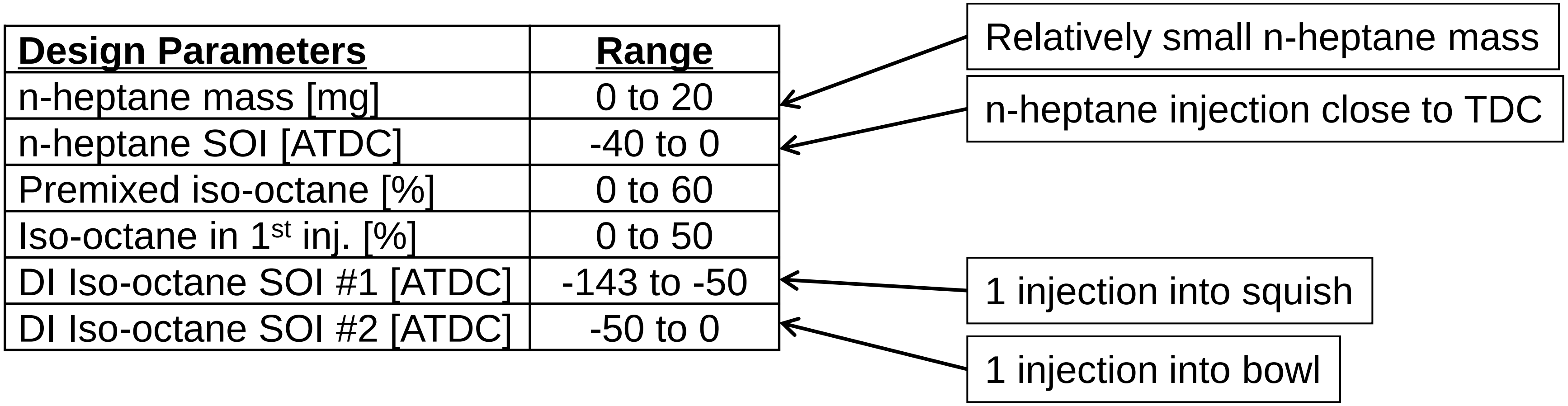
Large S:V ratio keeps the charge cooler near TDC

Additional fuel is injected in the bowl close to TDC

Lim, 2014

Extending RCCI load range

- Use NSGA (Nondominated Sorting Genetic Algorithms) II search-based global optimization tool
  - Searching for designs of 6 parameters to reduce 6 objectives:
    soot, NOx, CO, UHC, ISFC, and Ringing intensity
  - Total fuel mass: 245mg
  - 1800 rev/min



Design Parameters	**Range**
n-heptane mass [mg]	0 to 20
n-heptane SOI [ATDC]	-40 to 0
Premixed iso-octane [%]	0 to 60
Iso-octane in 1st inj. [%]	0 to 50
DI Iso-octane SOI #1 [ATDC]	-143 to -50
DI Iso-octane SOI #2 [ATDC]	-50 to 0

Relatively small n-heptane mass

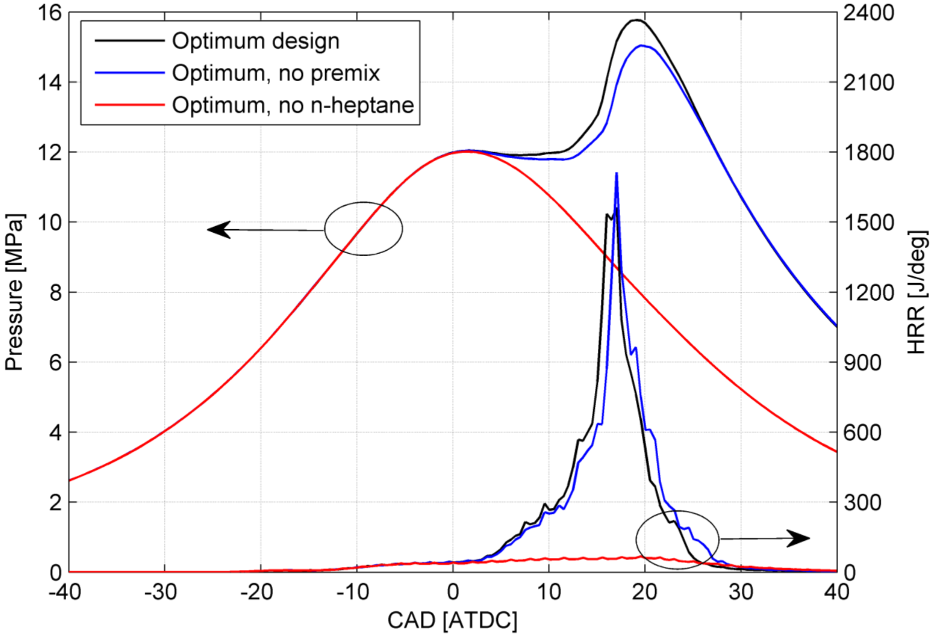
n-heptane injection close to TDC

1 injection into squish

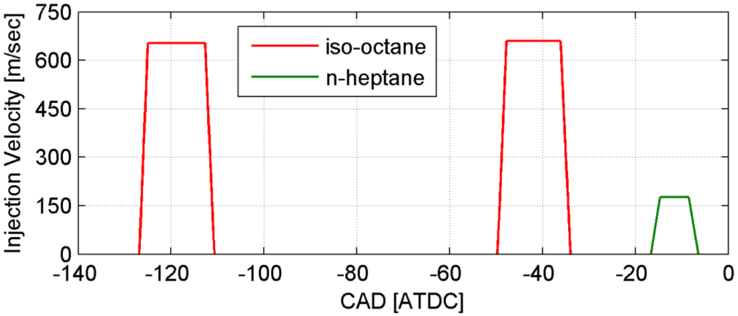
1 injection into bowl

Extending RCCI load range

GA search for optimum injection strategy



US 2010 Emission Targets
Soot: 0.01g/kW-hr
NOx: 0.26g/kW-hr

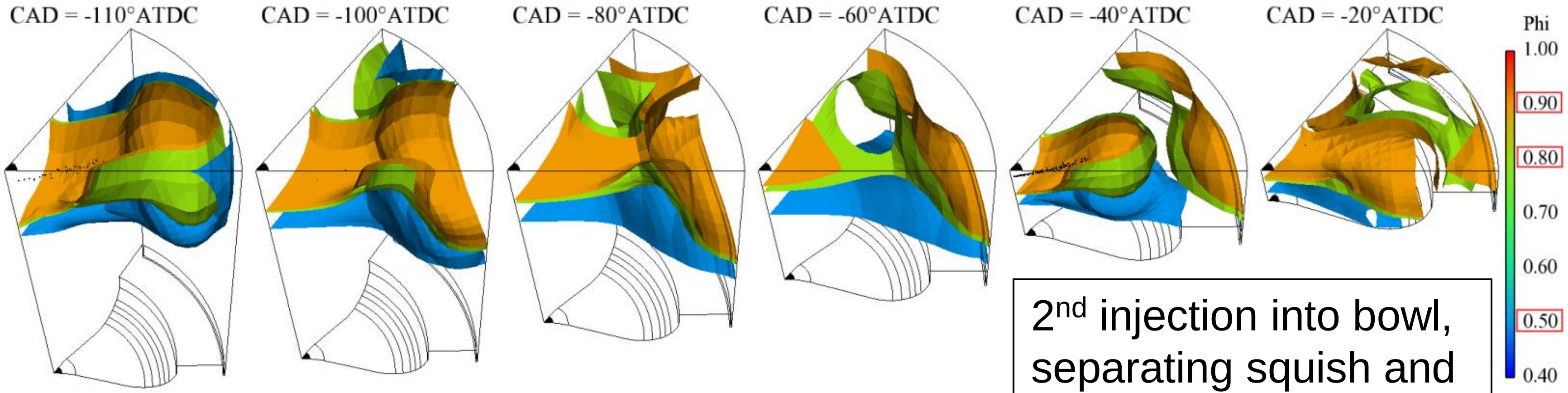


Optimum Design Parameters	
Premixed iso-octane mass [mg]	2.8
DI Iso-octane mass #1 [mg]	118.8
DI Iso-octane mass #2 [mg]	115.0
n-heptane mass [mg]	8.4
DI Iso-octane SOI #1 [ATDC]	-126.8
DI Iso-octane SOI #2 [ATDC]	-49.7
n-heptane SOI [ATDC]	-16.7

Soot [g/kW-hr]	0.015
NOx [g/kW-hr]	0.058
CO [g/kW-hr]	0.73
UHC [g/kW-hr]	1.13
ISFC [g/kW-hr, IVC→EVO]	174.7
η_g [%, BDC→BDC]	48.7
Ringing Intensity [MW/m^2]	10.2
PPRR [bar/deg]	12.6

Extending RCCI load range

Combustion control mechanism

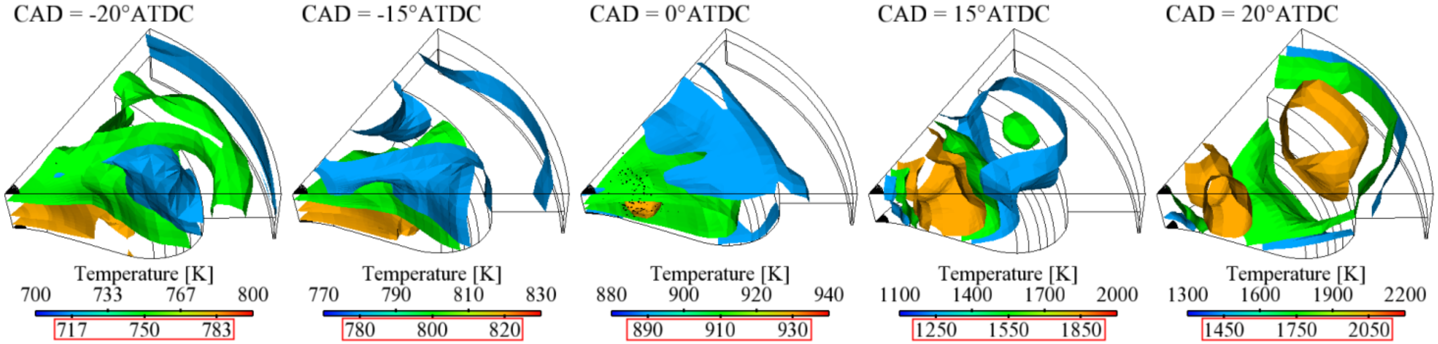


1st injection into squish

2nd injection into bowl, separating squish and bowl

Squish region remains cooler

Combustion starts from n-heptane. Squish combustion starts later

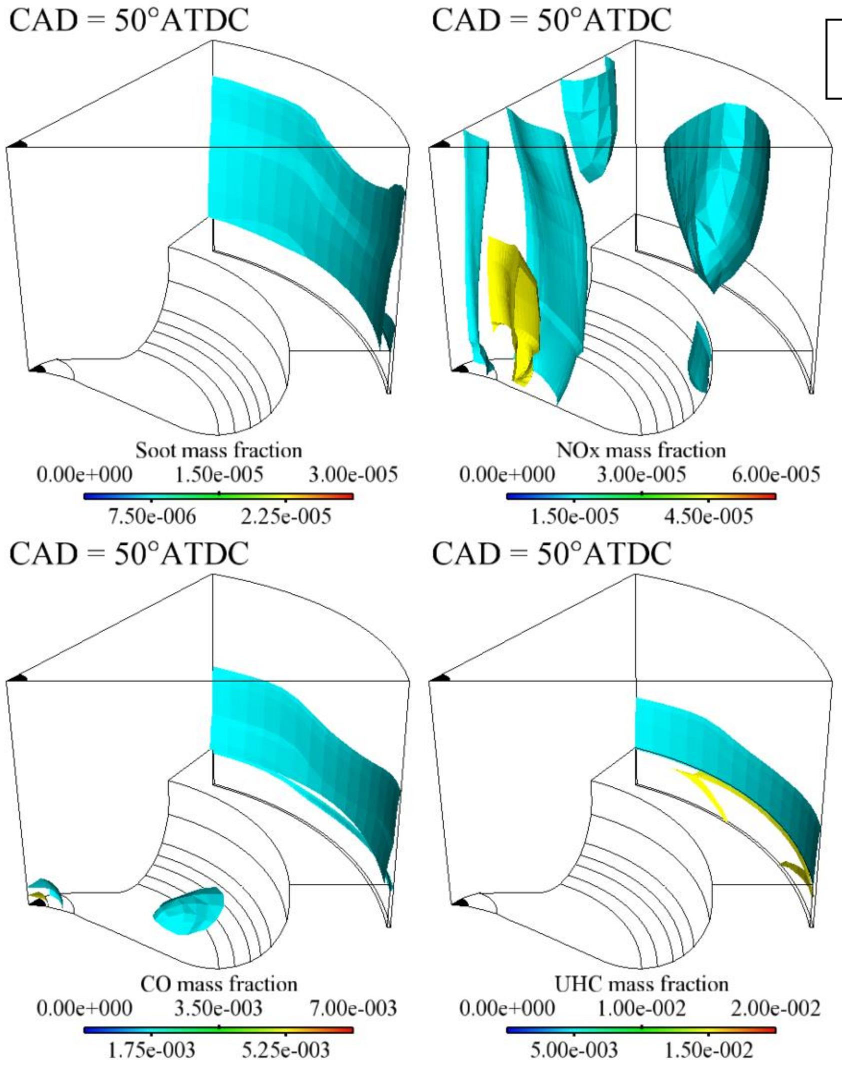


Extending RCCI load range

Source of emissions

Soot from liner

NOx from ignition site



CO from liner

UHC from ring pack crevice

Extending RCCI load range

Conclusions

- With 2 independent direct injectors RCCI combustion becomes possible at high load conditions.
- Larger mass of 1st iso-octane injection at -80°ATDC is most effective in squish “cooling.”
- 2nd injection timing sweeps show that earlier injection is more effective in lowering ringing intensity.
- n-heptane injection mass and timing is most effective for combustion control.
- Further study of piston geometry and injection direction is necessary.

Summary and conclusions

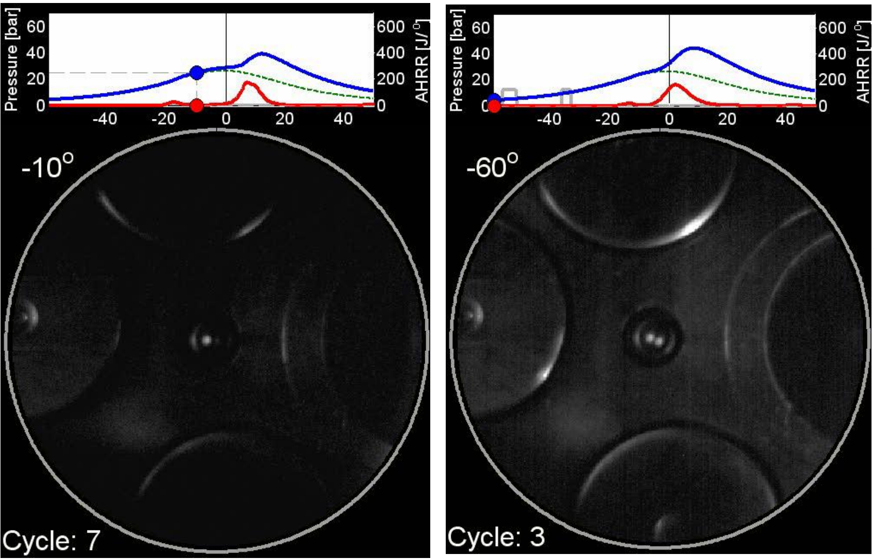
CFD modeling can be integrated with efficient optimization techniques for improved engine design

New combustion strategies can be discovered using CFD-optimization

Reactivity Controlled Compression Ignition strategy explained and validated with engine experiments

Dual fuel and single-fuel (with additive) RCCI provides combustion control using optimized blending of port- and direct-injected fuels

RCCI offers high thermal efficiency and meets EPA NOx and soot emissions mandates in-cylinder, without the need for after-treatment



HCCI

RCCI