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In-Cylinder Processes of Natural Gas Combustion Modes

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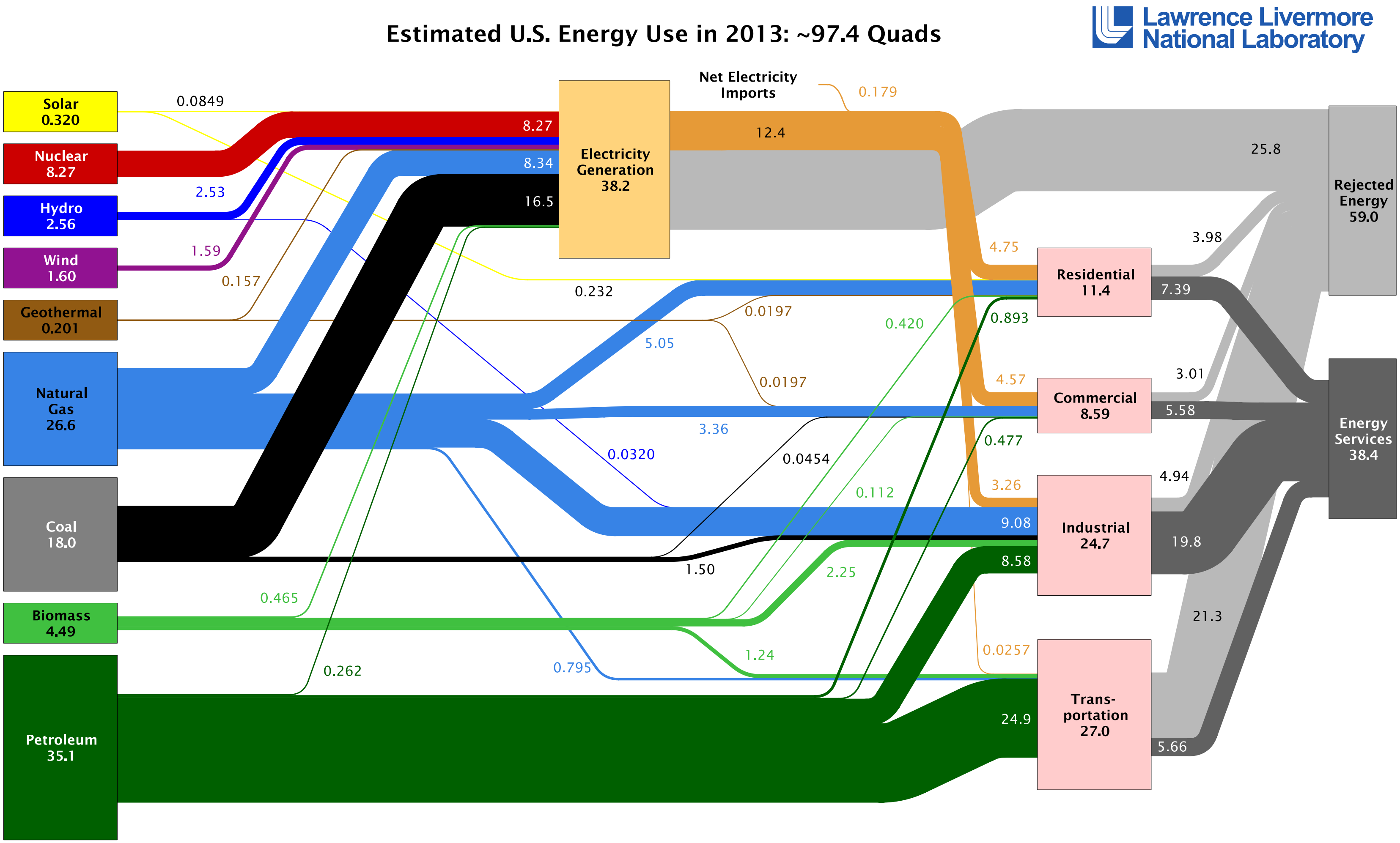
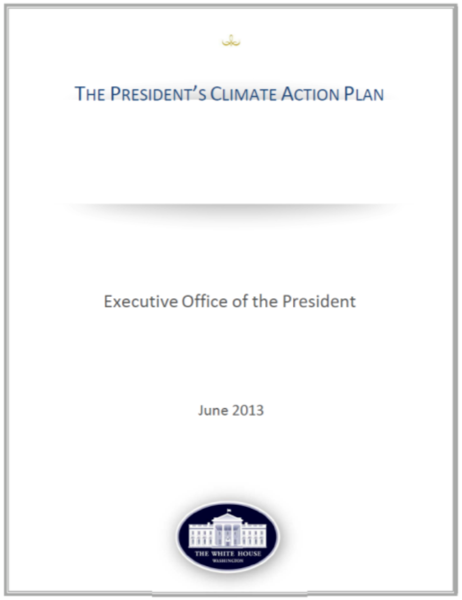
Program Managers: Gurpreet Singh, Leo Breton, Kevin Stork

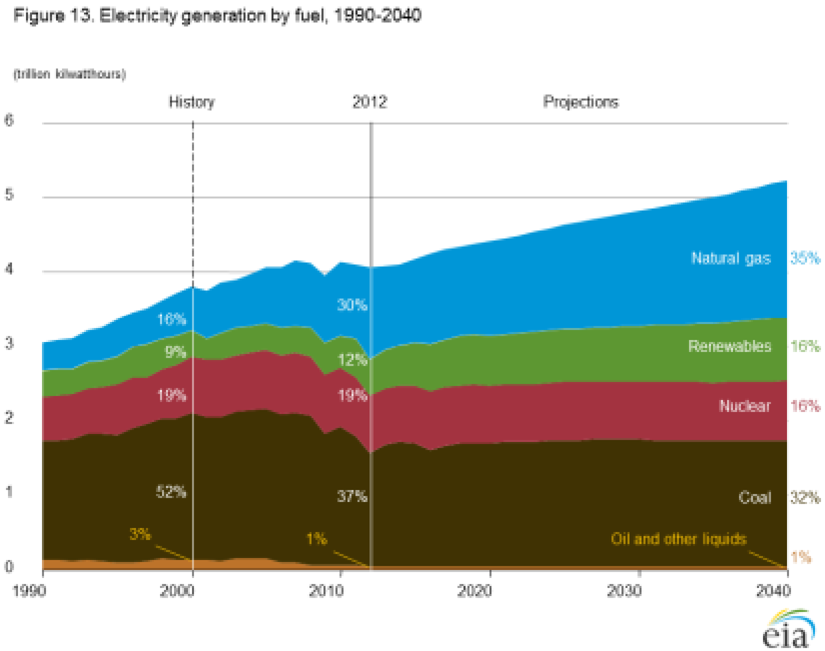
US 2013: total NG prod. ≅ total transport energy, but NG ~3% of transport (EU28: 0.8%, China~1%)



Source: LLNL 2014. Data is based on DOE/EIA-0035(2014-03), March, 2014. If this information or a reproduction of it is used, credit must be given to the Lawrence Livermore National Laboratory and the Department of Energy, under whose auspices the work was performed. Distributed electricity represents only retail electricity sales and does not include self-generation. EIA reports consumption of renewable resources (i.e., hydro, wind, geothermal and solar) for electricity in BTU-equivalent values by assuming a typical fossil fuel plant "heat rate." The efficiency of electricity production is calculated as the total retail electricity delivered divided by the primary energy input into electricity generation. End use efficiency is estimated as 65% for the residential and commercial sectors 80% for the industrial sector, and 21% for the transportation sector. Totals may not equal sum of components due to independent rounding. LLNL-MI-410527

US goals for emissions/GHG reduction promote increased NG for electricity & transportation

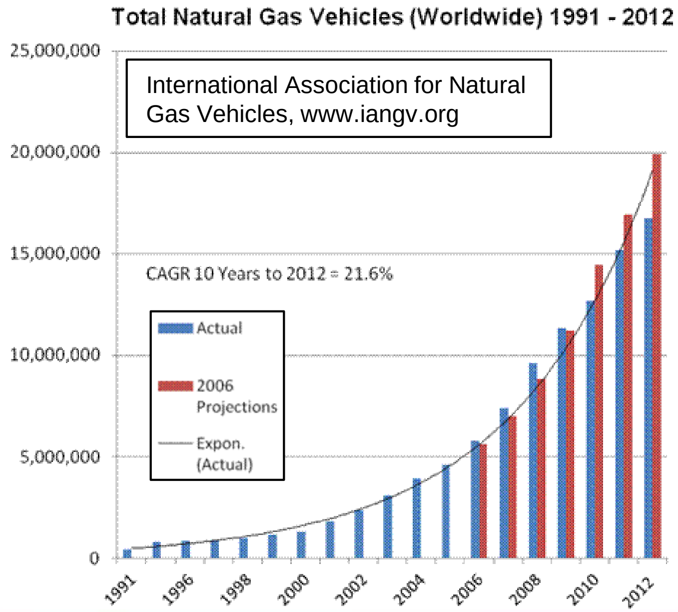


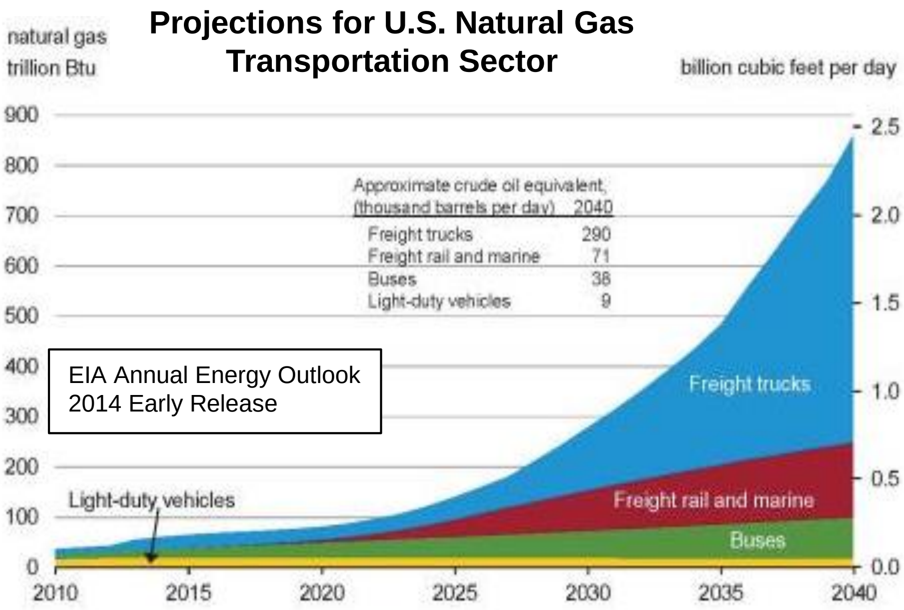


- Climate Action Plan – Promote fuel switching from oil & coal to NG
  - Produces 50% less CO_2, a third of the NO_x, 1% SO_x relative to coal for power
  - NG combustion at >50% of new electricity generation, push for greater usage
- Transport cost incentive – Tax increase Prevention Act of 2014 (H.R. 5771)
- US DOE Vehicle Technologies Office – Promote technologies that reduce petroleum use while lowering costs and reducing environmental impacts
  - NG 6-11% lower GHG relative to gasoline (DOE Alternative Fuels Data Center)
  - Renewable NG up to 88% lower GHG (ANL Waste-to-Wheel Analysis)

World NGVs growth +20% annual, largely light-duty; US projected growth (~10%) is mostly heavy duty

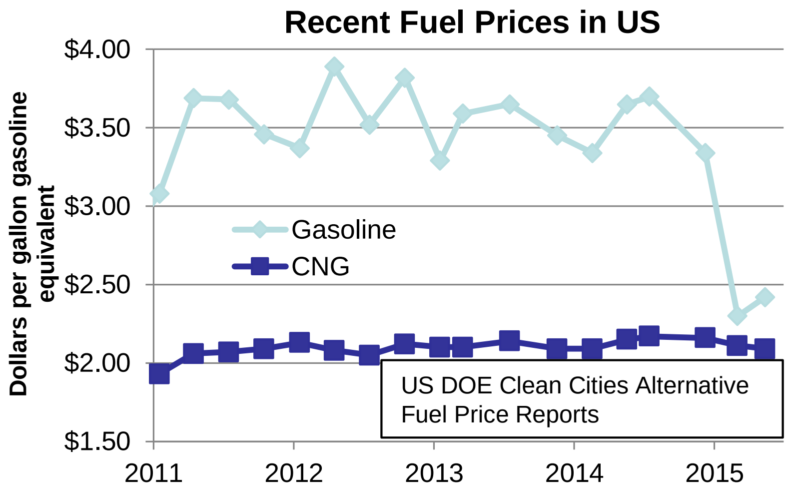
- IANGV: 2012 worldwide NG vehicles (NGV) at 16.7M (1.3% of total vehicles)
  - #1 Iran (3M-21%) #2 Pakistan (2.9M-65%) #3 Argentina (2.1M-17%) #4 Brazil (1.7M-3.6%) #5 China (1.6M-1.1%) #6 India (1.3M-1.5%) #7 Italy (750k-1.6%) #18 USA (130k-0.05%) #19 Germany (95k-0.19%) #23 Sweden (44k-0.84%) #24 Japan (43k-0.06%) #25 Korea (34k-0.18%) #28 France (13k-0.03%) #29 Canada (13k-0.06%) #30 Switzerland (11k-0.21%)
- NG passenger car market in US is relatively small with little growth anticipated, but rapid (~10% annual) growth is expected in heavy-duty, bus, rail, and marine markets

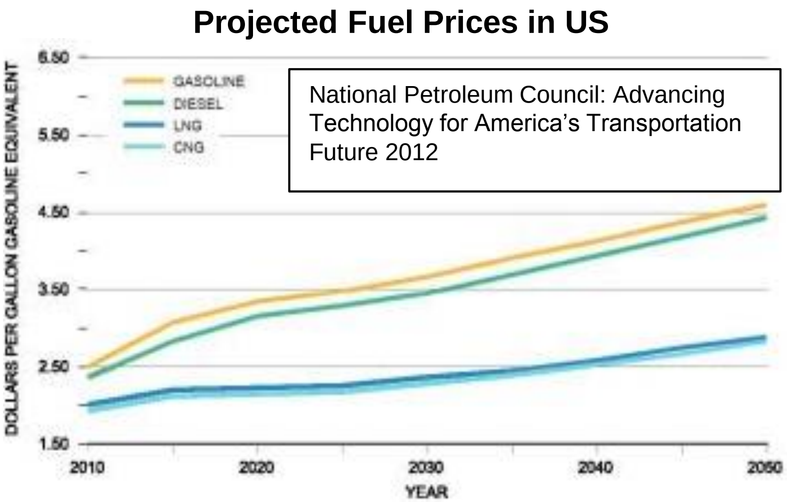




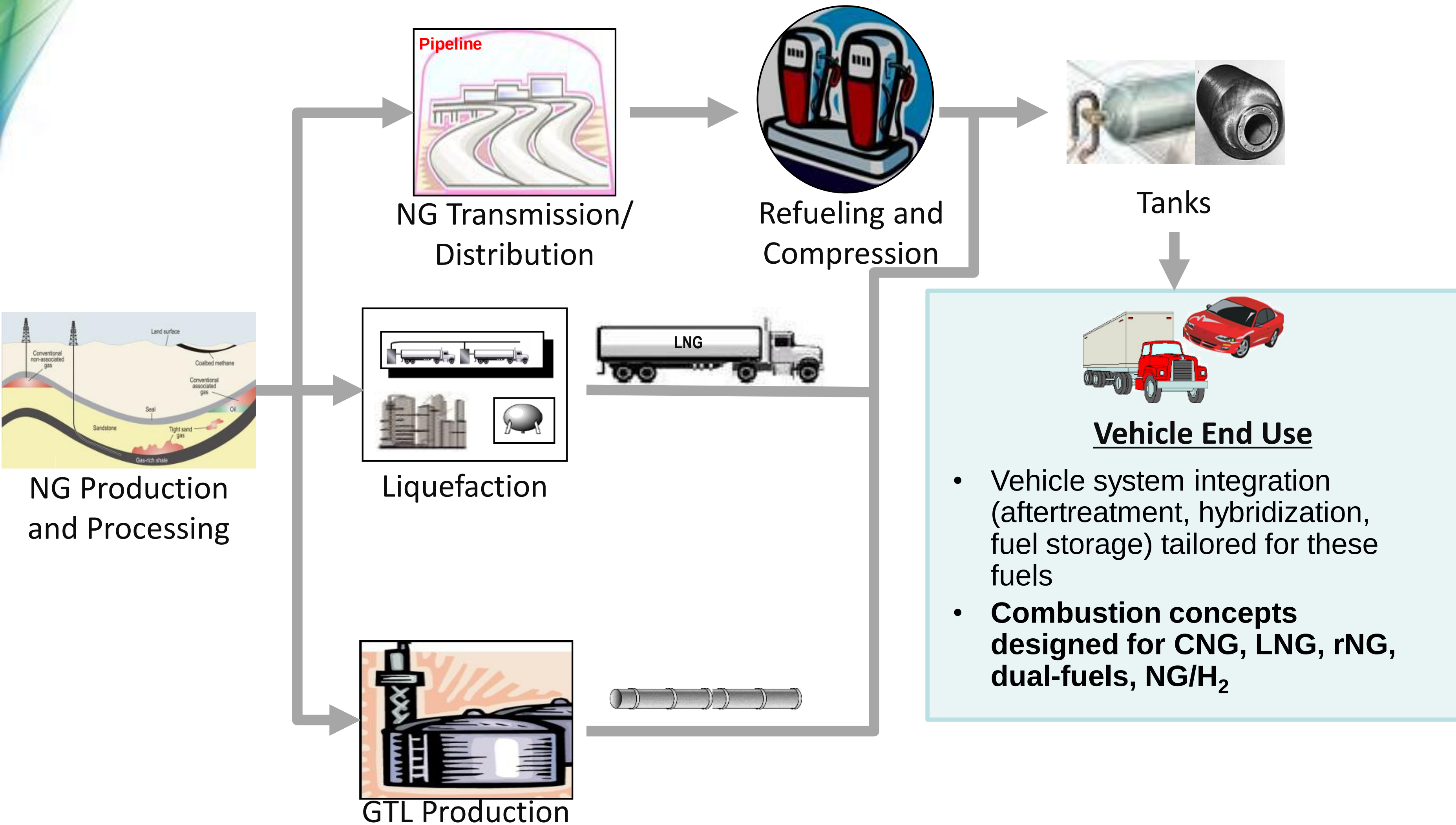
Projected increased NG usage in US heavy-duty transportation market driven by economics

- Since 2011, US NG prices have been consistently lower than gasoline/diesel
  - But transportation fuel costs are not strong driver for US passenger car market; US drivers pay among lowest unit fuel costs relative to income (in 2014, ~2% of daily wage per gallon in US, median is 9.6% - Bloomberg)
  - Fuel costs are more important in heavy-duty on-road and rail transport (~40% of operating costs – American Transportation Research Institute)
- Recent NG production gains due to hydraulic fracturing and shale gas development are projected to maintain a large price differential in the US through 2060



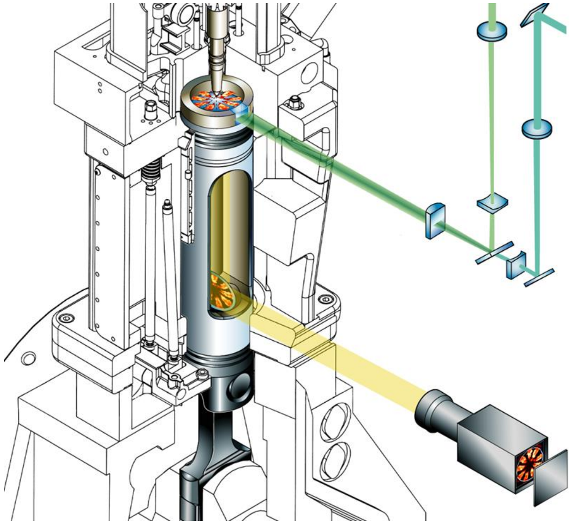


Improvements are needed at many steps in NG supply chain – Sandia/CRF focus is combustion



US Summary: Optical engine research to provide a science base to overcome NG end-use barriers

- Current NG supply/economics: R&D to improve NG usage in heavy-duty engines responds to both the push from USDOE and the economic pull from domestic industry
- Key R&D areas:
  - Distribution/refueling
  - GTL/LNG production
  - On-board storage
  - **Vehicle end-use**
- Four NG engine combustion strategies in production:
  - "Best" combustion strategy depends on economics/regulations/performance
  - Each faces unique challenges
  - Much less optical engine data available for NG compared to liquid fuels

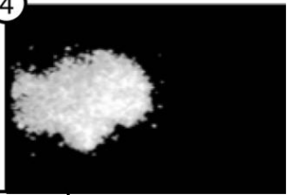


Common-platform optical engine can provide missing science base

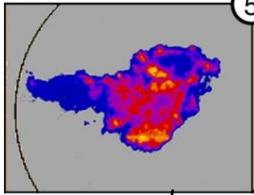
Optical engine led to diesel "conceptual model"; Is now industry standard for conventional diesel

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

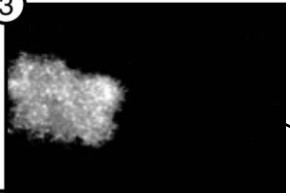
PAH PLIF: Soot Precursors (4)
As hot ignition reactions increase the temperature in the jet, fuel fragments are formed into chemical building blocks for soot.



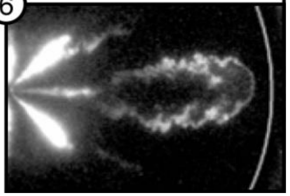
LII: Soot Concentration (5)
Shortly after the premixed fuel burns, soot is formed in the hot, fuel-rich region throughout the jet cross-section.



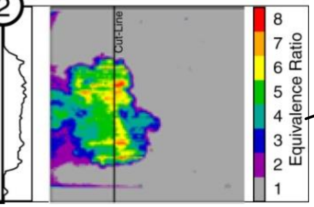
Chemiluminescence: Ignition (3)
Spontaneous ignition reactions occur in the hot mixture of fuel and air throughout the leading portions of the jet.

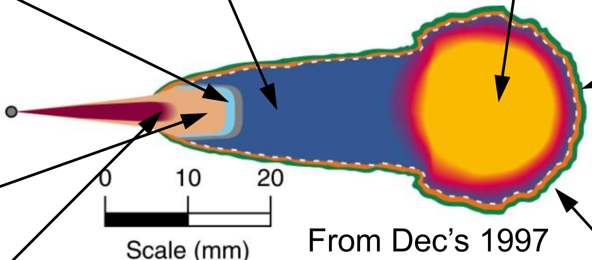


OH PLIF: Diffusion Flame (6)
Shortly after the premixed fuel burns, a thin diffusion flame forms on the jet periphery, surrounding the interior soot cloud.



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

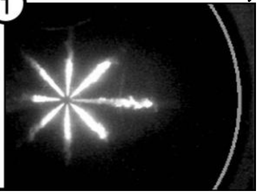




From Dec's 1997 conceptual model (SAE 970873)

NO PLIF: Thermal NO (7)
NO forms on the periphery of the jet in the hot diffusion-flame products.

Mie Scatter: Liquid Fuel (1)
After penetrating approx. 25 mm, the hot, entrained gases completely vaporize the liquid fuel.



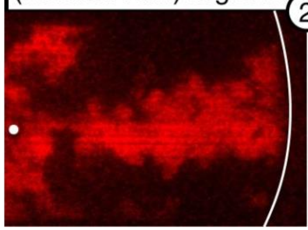
Liquid Fuel
Rich Vapor-Fuel/Air Mixture
Diffusion Flame
Fuel-Rich Premixed Flame
Initial Soot Formation
Thermal NO Production Zone
Soot Oxidation Zone

Low — High
Soot Concentration

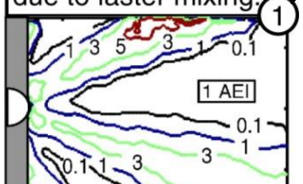
First conceptual model motivated new strategies;
↳ New low-temperature diesel conceptual model

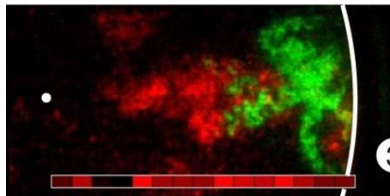
O_2 = 13% (high EGR)
SOI = 22 BTDC
P_{inj} = 1200 Bar

H_2CO PLIF: 1st-Stage Ignition
Formadehyde appears nearly simultaneously in the jet, from fuel-lean (upstream) to fuel-rich (downstream) regions. (2)



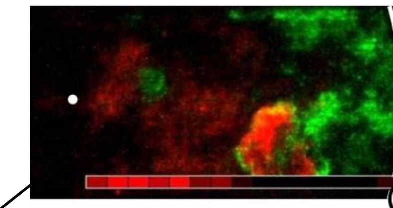
Fuel-Tracer PLIF: Φ
After fuel injection, equivalence ratios decrease and liquid fuel vaporizes rapidly due to faster mixing. (1)



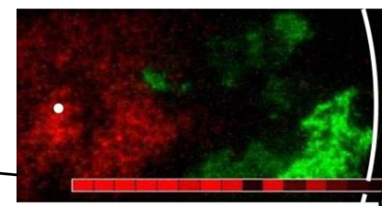


(3) **OH PLIF: 2nd-Stage Ignition**
OH (green) appears downstream, in wide bands distributed over the width of the jet. Formaldehyde (red) remains upstream.

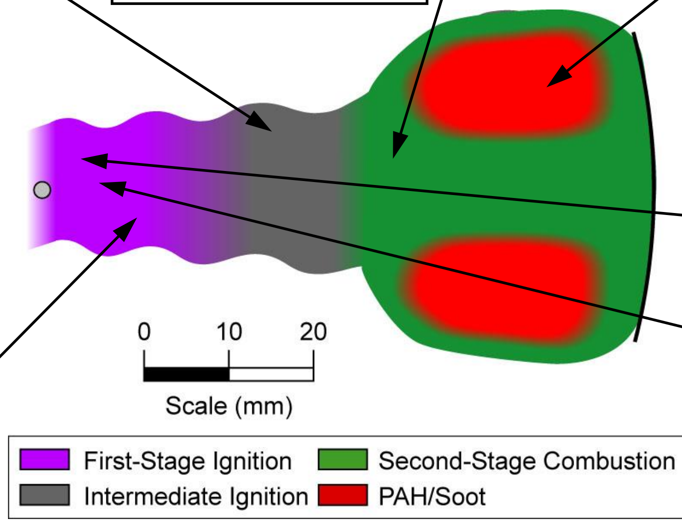
From 2013 LTC conceptual model (PECS 39:246-83)

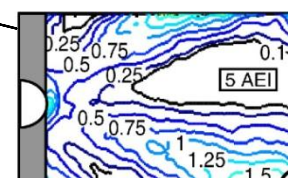


PAH PLIF: Soot Precursors
PAH species (bright red) form near the jet head-vortex, where adjacent jets interact. Formaldehyde (dim red)
(4) still remains, upstream.



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

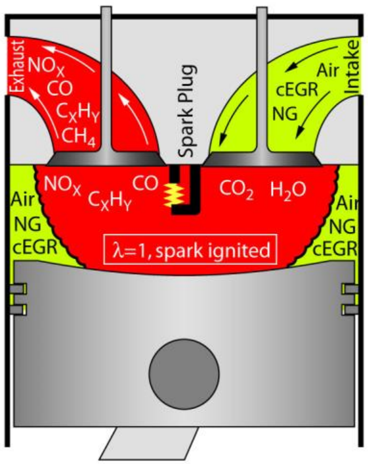




Fuel-Tracer PLIF: Φ
During ignition delay, near-injector mixtures become too fuel-lean to burn completely,
(6) leading to unburned HCs.

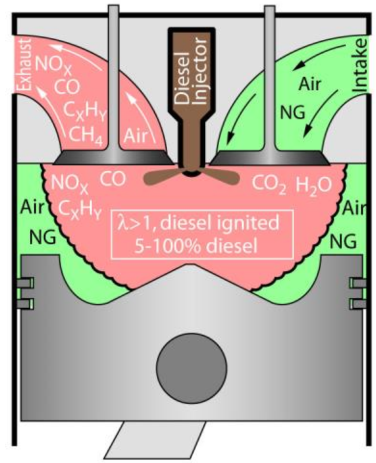
Four production NG combustion strategies today; balance of economics, regulation, & performance

Spark/Prechamber Ignition



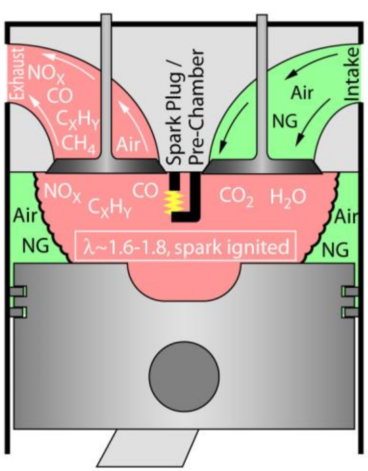
Stoichiometric Spark Ignition

- Premixed intake, NG+air+cEGR
- 3-way catalyst
- ~36% efficiency
- 100% NG
- Cummins, Scania, Waukesha, IVECO



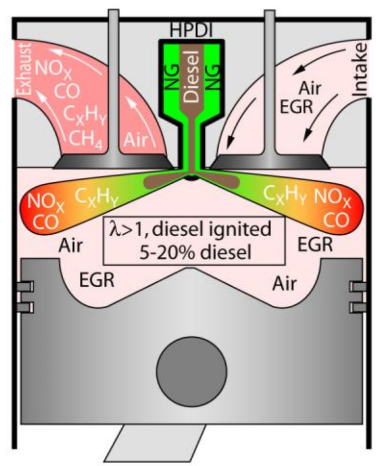
Lean Premixed Diesel Pilot

- Premixed intake, NG+air+cEGR
- Oxy-catalyst
- ~45% efficiency
- 0-95% NG
- Volvo (Hardstaff, G-Volution retro.)



Lean Premixed Spark Ignition

- Premixed intake, NG+air+EGR
- Oxy-catalyst
- ~44% efficiency
- 100% NG
- Cummins, MAN, Doosan, GE



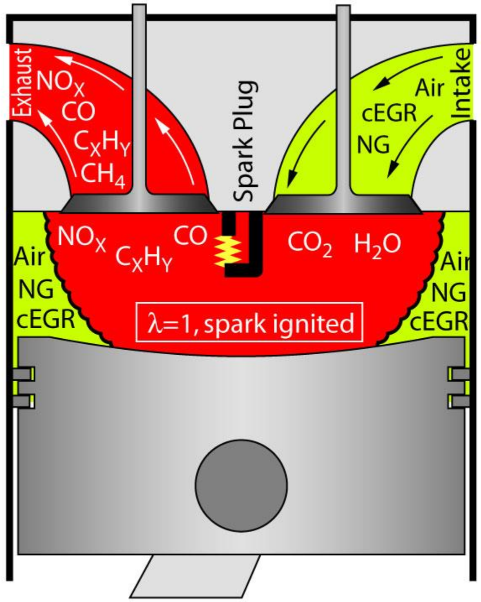
Direct Injection Diesel Pilot

- intake: air + EGR
- Catalyzed DPF, Urea SCR
- ~46% efficiency
- ~90% NG
- Westport, Volvo

Diesel-Pilot Ignition

Each NG strategies faces unique combustion challenges

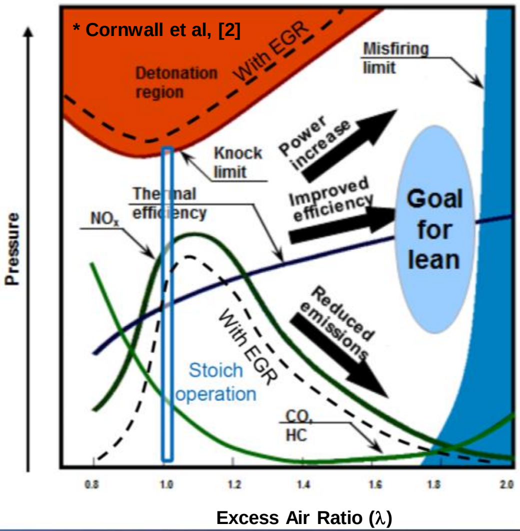
Stoichiometric spark-ignition challenges include efficiency, fuel variability, and knock/load limits



Intake	Premixed NG, Stoichiometric	Methane-specific 3-way catalyst for CO, HC, NOx[2]
	Cooled EGR	Reduces NOx & heat load, raises knock limit[1,2]
Fuel Efficiency	Low (~36%)[1]	Throttle, Timing Retard, EGR + low compression ratio to avoid knock[1]
NG Fraction	100%[1,2]	No diesel fall-back[2]
Key HD Dev.	Cummins, Scania, Waukesha, IVECO[2]	

In-cylinder gaps for NG stoichiometric/EGR spark ignition

- Controlling flame kernel/growth/knock transition[1]
  - Surface/geometry effects
  - Fuel composition effects
  - EGR/fuel mixing/distribution effects[1]
- Using turbulence to increase flame speed with EGR
  - Effects on ignition, misfiring issues[1]



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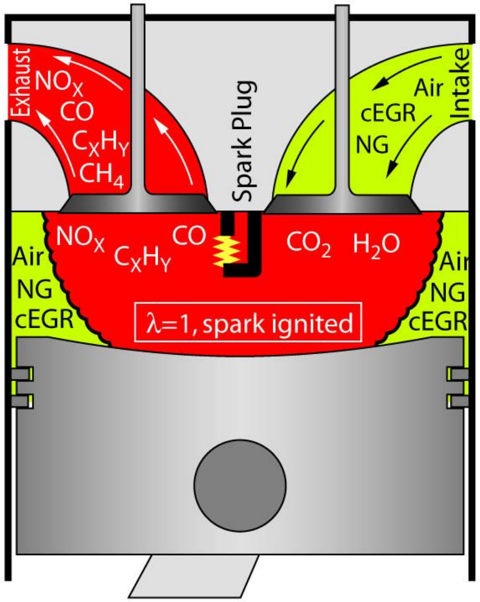

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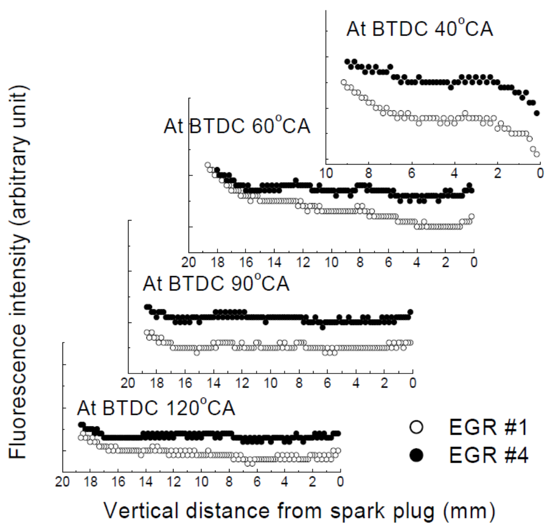
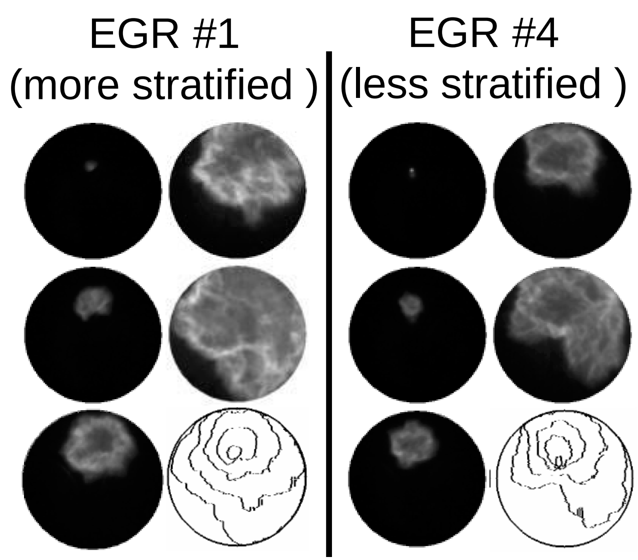
Previous optical work:

- With LPG, intake port valve can place EGR in bottom of cylinder
- More stratified EGR burns faster and with higher efficiency

* SAE 2004-01-0928, Woo, Yeom, Bae (KAIST); Oh, Kang (KIMM)





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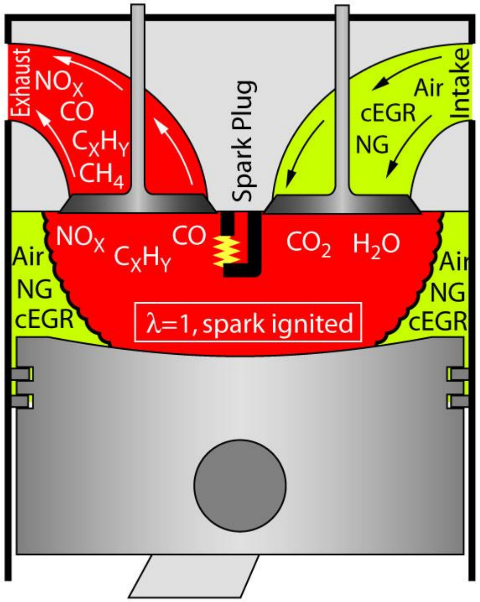

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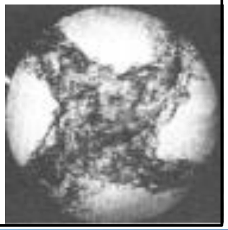
Understand factors that control NG knock with EGR

- Kernel/flame growth
- Surfaces/geometry
- Fuel composition (inc. H_2)
- EGR distribution
  - Mixing diagnostics

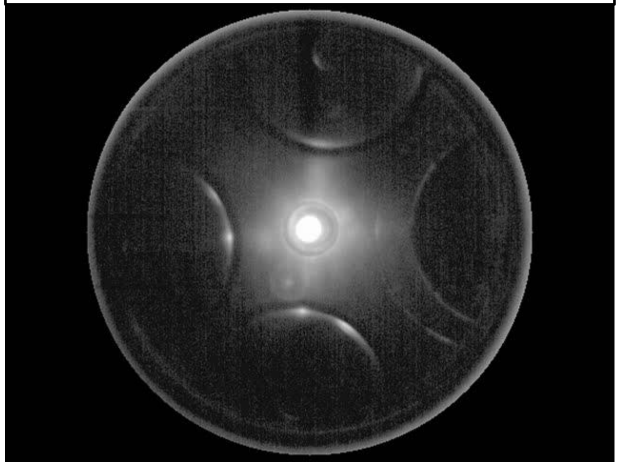
Schlieren images of knocking combustion

Prior to autoignition of end-gas

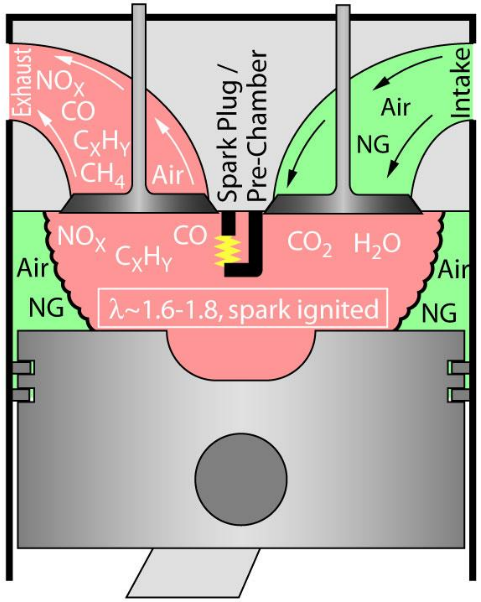
Onset of knocking



High-speed chemiluminescence imaging of knock-free combustion



Lean premixed spark-ignition challenges include ignition stability, transients, and CH_4 slip



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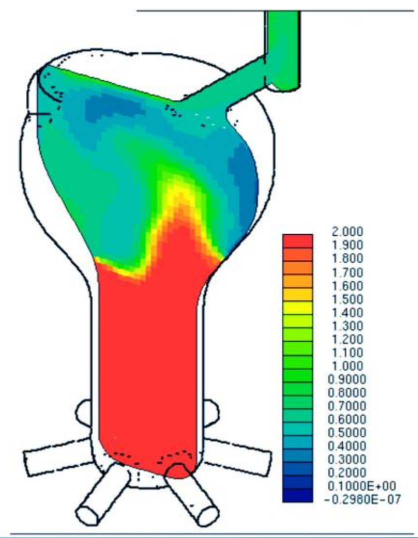
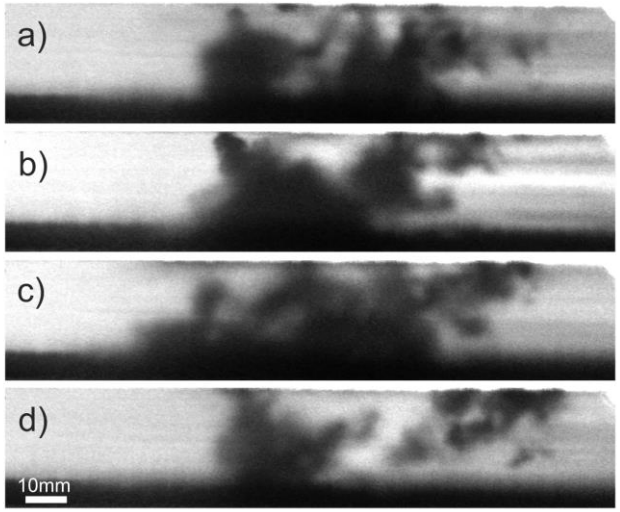
Efficiency	~44%	high specific heat ratio, high compression ratio
Heavy-Duty	Cummins, Scania, MAN, GE (Jenbacher)	
Challenges	Ignition stability (pre-chamber), transients, SCR for US2010/Euro VI NOx, CH_4 slip (low exhaust T / catalyst-efficiency)	

Pre-chamber simulation



Acetone PLIF: fuel consumption



Previous optical work:

- PLIF shows pre-chamber stratification, comp. inflow
  - Variability lowers knock limit
- Pre-chamber-jet mixing increases flame speed

* SAE 2014-01-1330 Wellander, Rosell, Richter, Alden, Andersson, Johansson (Lund); Duong, Hyvonen (Wartsila)

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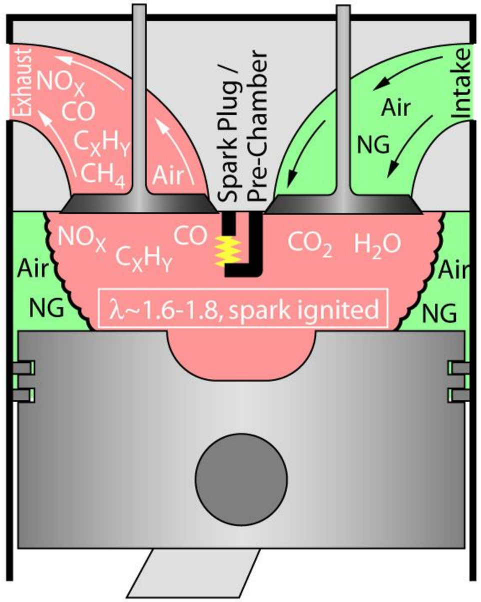

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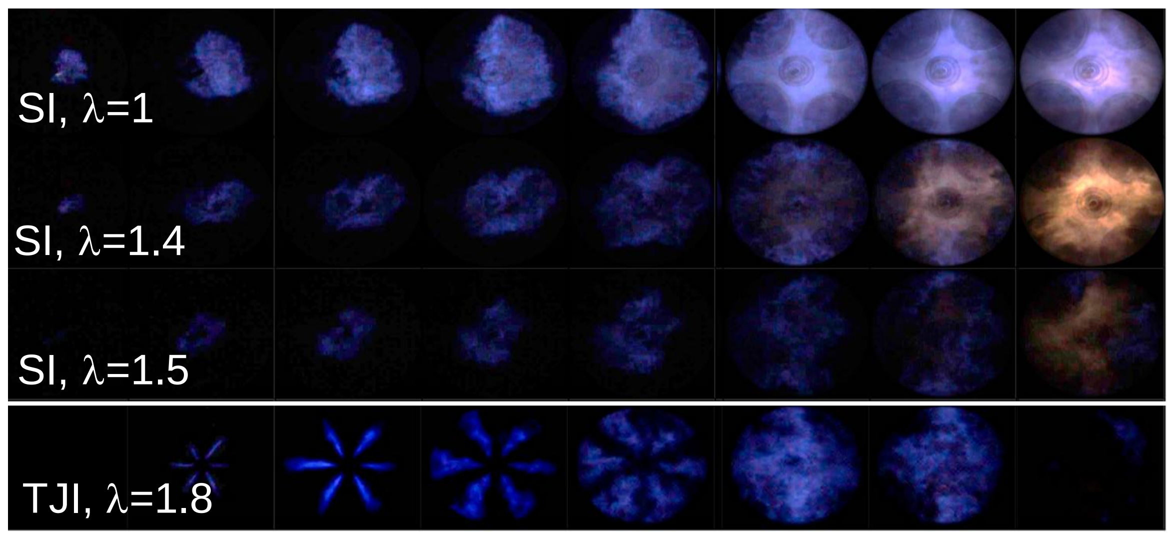
Natural Luminosity imaging

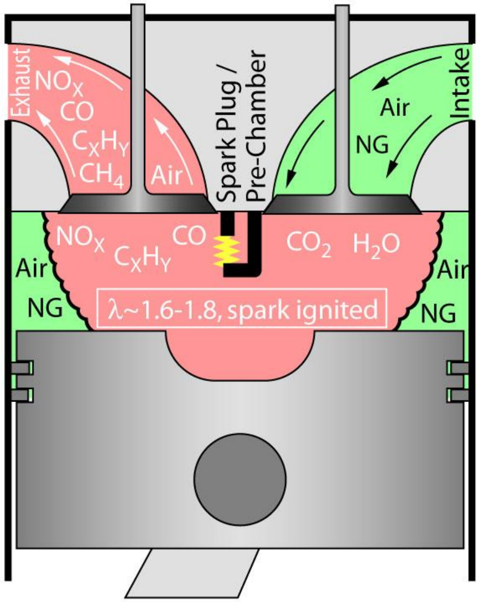


<u>Previous optical work:</u>

- Turbulent jet ignition pre-chamber allows leaner operation with higher stability & combustion efficiency

*SAE 2012-01-0823, Attard (MAHLE); Toulson, Huisjen, Chen, Zhu, Schock (Michigan State U)

Lean premixed spark-ignition challenges include ignition stability, transients, and CH_4 slip



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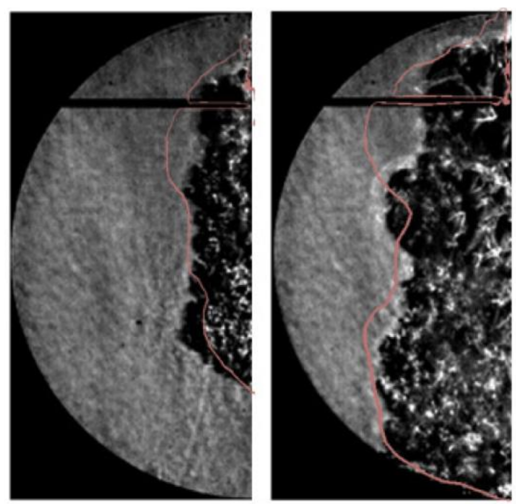
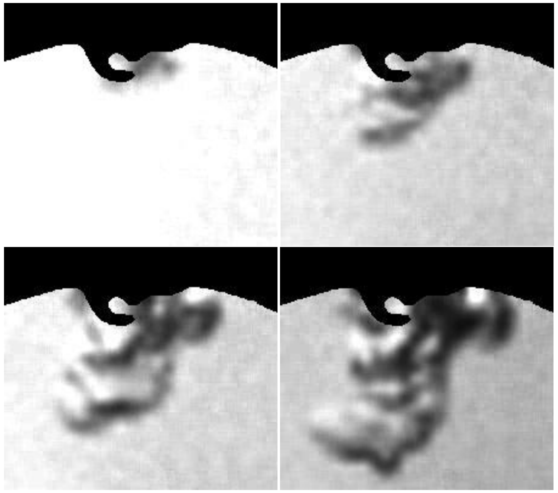
Schlieren spark-ignited jet*



Schlieren jet-capillary spark plug**

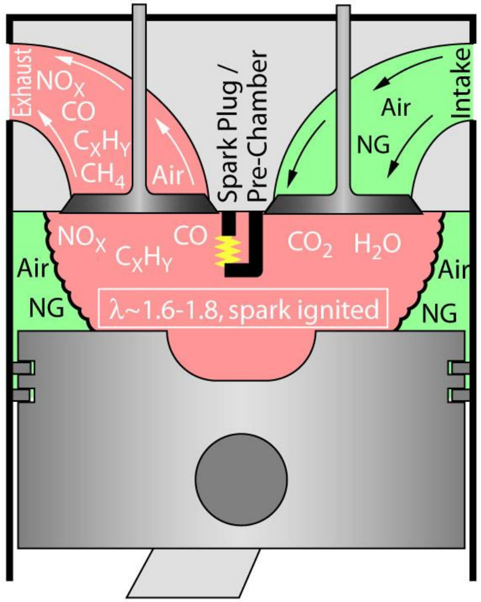


Previous optical work:

- Spark-ignited jets improve combustion speed/stability at overall lean conditions

* SAE 2015-01-0398, Bartolucci, Cordiner, Mulone, Rocco (Rome Tor Vergata); Chan (U British Columbia)
** SAE 2007-01-1913, Chan, Evans, Davy (U British Columbia); Cordiner (Rome Tor Vergata)

Lean premixed spark-ignition challenges include ignition stability, transients, and CH_4 slip

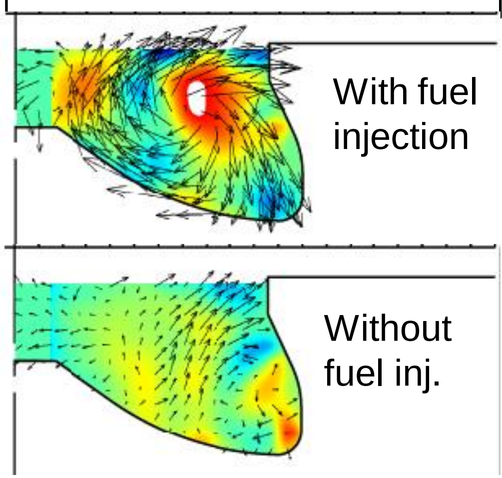


Intake	Lean-premixed NG (λ~1.6-1.8)	Aftertreatment for HC and CO only
Efficiency	~44%	high specific heat ratio, high compression ratio
Heavy-Duty	Cummins, Scania, MAN, GE (Jenbacher)	
Challenges	Ignition stability (pre-chamber), transients, SCR for US2010/Euro VI NOx, CH_4 slip (low exhaust T / catalyst-efficiency)	

Understand fuel-lean flame ignition/propagation issues

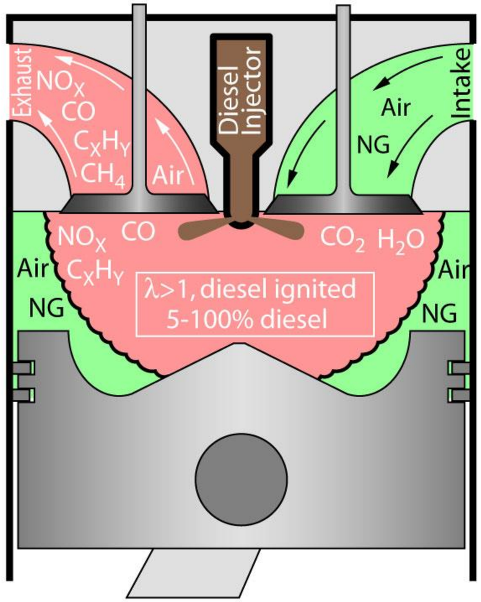
- Lean spark/pre-chamber ignition kernel growth
- Flow/piston-geometry interactions
- Incomplete combustion
  - Fuel/tracer diagnostics

Particle Image Velocity Measurements



High-speed chemiluminescence imaging of RCCI with laser spark

Lean premixed diesel-pilot ignition challenges include combustion efficiency, aftertreatment cost



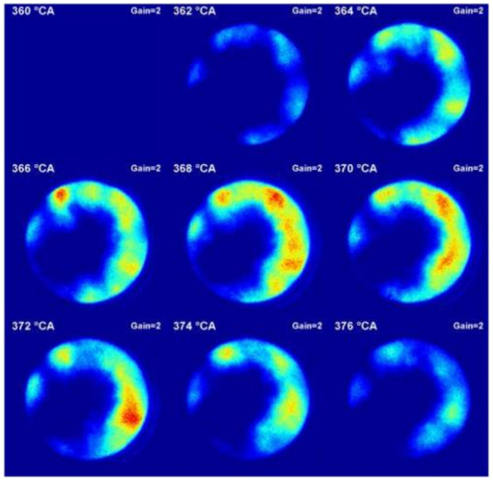
Intake	lean-premixed NG + EGR	aftertreatment for HC and CO, possibly NOx
Efficiency	~45%	high specific heat ratio, high compression ratio
NG fraction	0-95%	can run 100% diesel
Heavy-Duty	Volvo; retrofit: CAP, Hardstaff, G-Volution	
Challenges	combustion efficiency (CO, CH_4), aftertreatment costs	

Previous optical work:

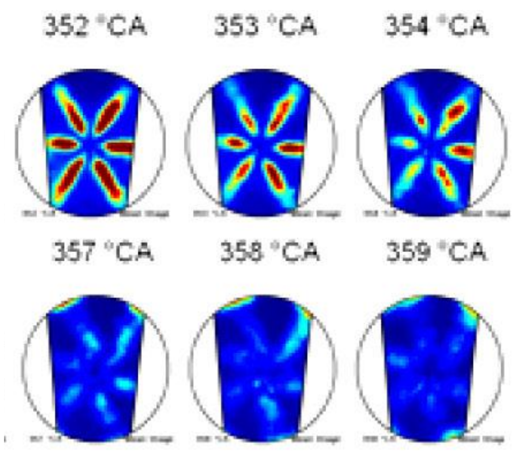
- OH Chemiluminescence shows bowl-wall ignition, incomplete combustion at center for low ϕ
- Fuel-tracer PLIF: fuel-lean at center, akin to diesel LTC PCCI

*SAE 2014-01-1313, Dronniou, Kashdan, Lecointe (IFPEN); Sauve, Soleri (Westport Innovations)

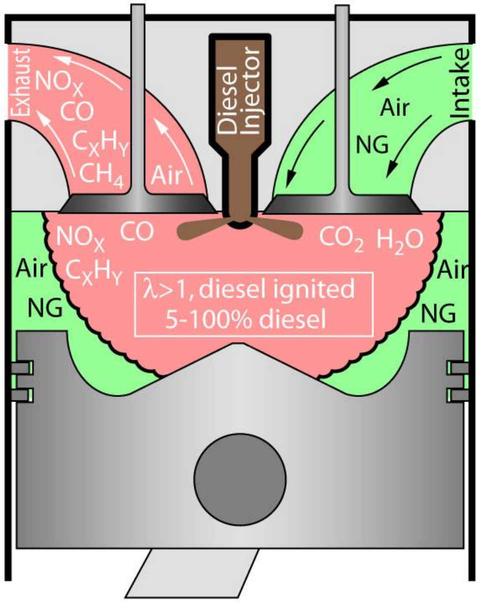
OH Chemiluminescence



Fuel-tracer PLIF



Lean premixed diesel-pilot ignition challenges include combustion efficiency, aftertreatment cost



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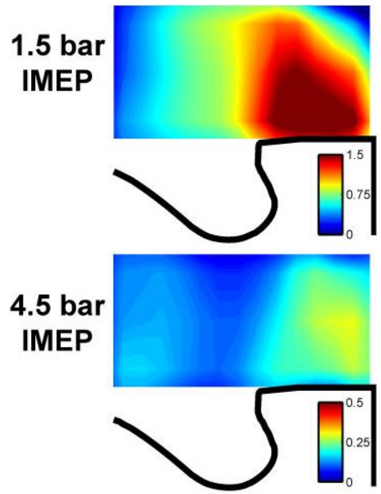
Challenges	combustion efficiency (CO, CH_4), aftertreatment costs	

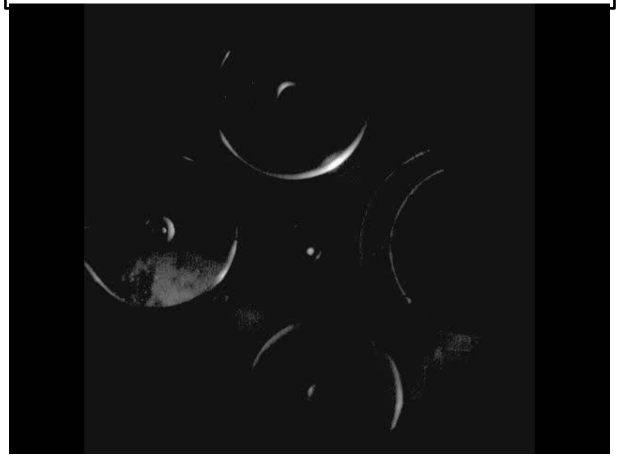
Understand fuel-lean NG w/ diesel-pilot ignition issues

- Source of CO (lean/rich)
  - Fluorescence/absorption
- Incomplete combustion
  - CH_4/Intermediates
- Source of NO (pilot comb.)

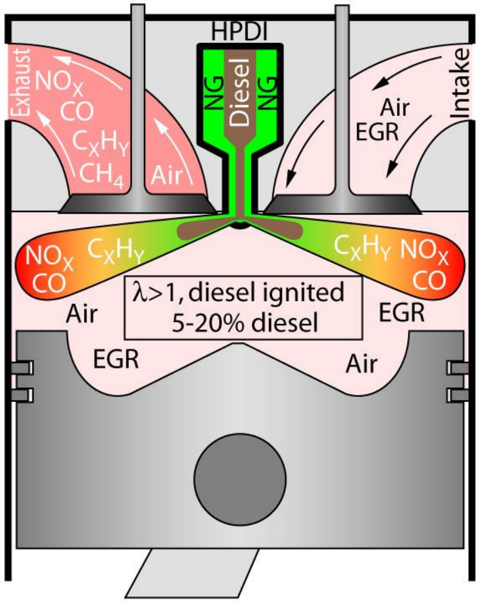
CO Fluorescence Images



High-speed chemiluminescence of premixed gasoline + diesel



High-pressure direct injection challenges include diesel aftertreatment cost, injection interactions

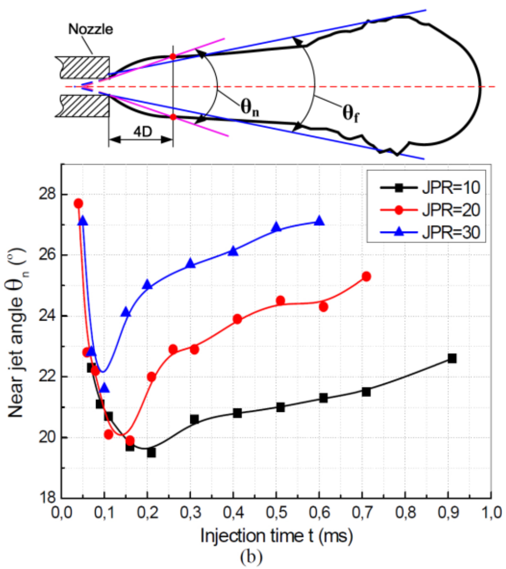


Intake	air + EGR	DPF + Urea SCR (diesel)
Efficiency	~46%	high specific heat ratio, high compression ratio
NG fraction	80-95%	can't run 100% diesel
Heavy-Duty	Volvo; retrofit: CAP, Hardstaff, G-Volution	
Challenges	Diesel-like emissions, optimize dual inj.	

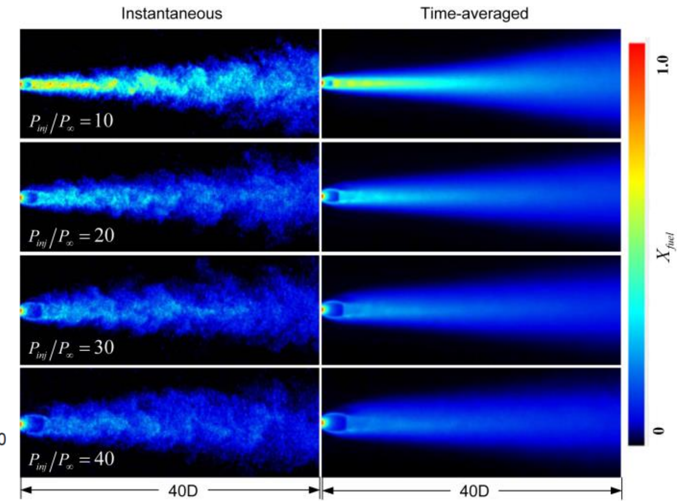
Previous optical work:

- PLIF shows pressure ratio affects shock structures and spreading angle & volume
- Shock-induced turbulence enhances mixing

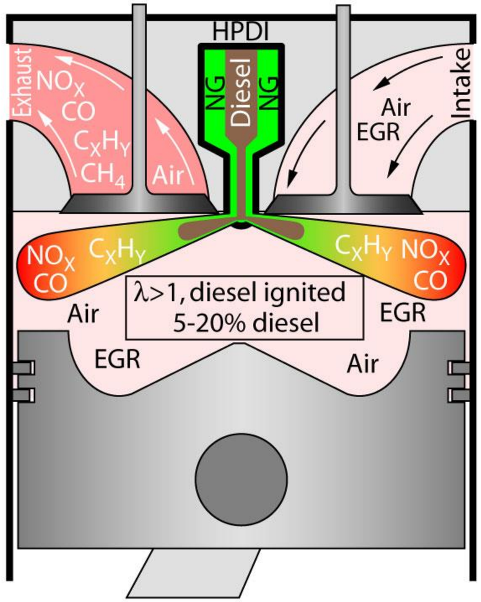
* SAE 2014-01-1619 Yu, Vuorinen, Kaario, Sarjovaara, Larmi (Aalto)



Acetone PLIF: N_2 jet in chamber



High-pressure direct injection challenges include diesel aftertreatment cost, injection interactions



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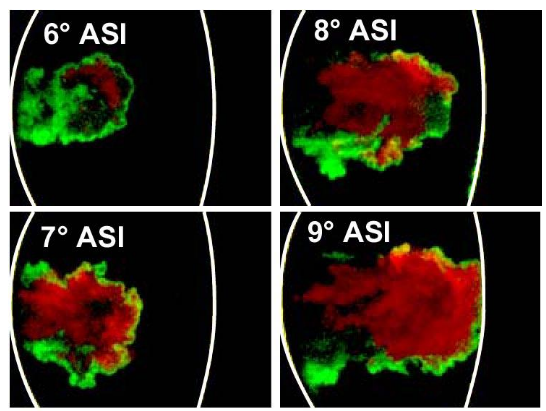
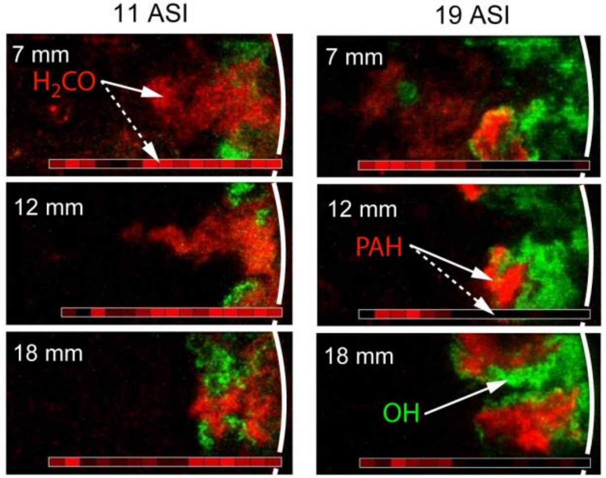
Challenges	Diesel-like emissions, optimize dual inj.	

Diesel: combined soot PLII (red) and OH PLIF (green)



Diesel LTC: combined HCO/PAH PLIF (red) and OH PLIF (green)



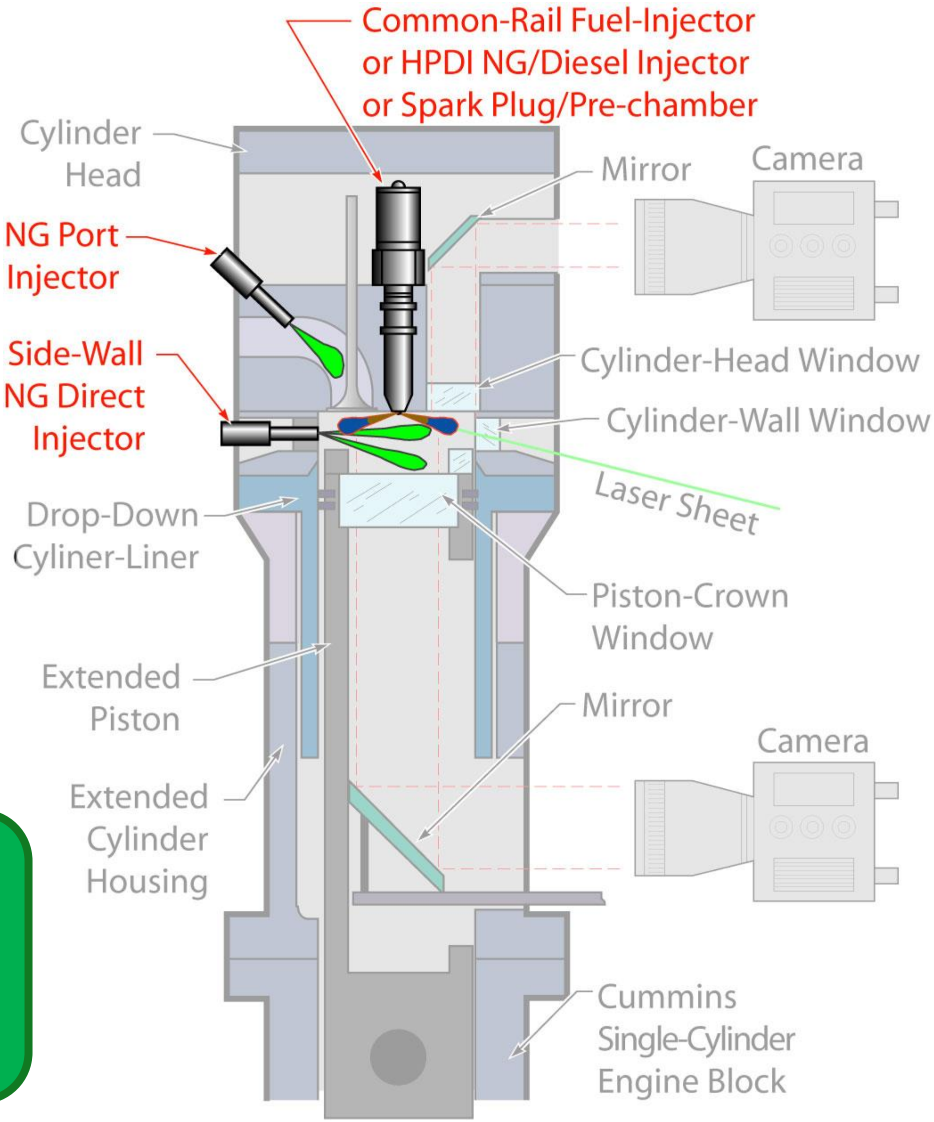
Understand high-pressure direct-injection NG issues

- Flame lift-off with NG and diesel pilot ignition
  - OH LIF/chemiluminesc.
  - Soot LII / PAH LIF
- Explore LTC options
  - Partial premixing

Adapting heavy-duty optical diesel engine for NG to provide common platform, 4(+) comb. strategies

Some industry perspectives:

- "A comprehensive optical dataset would be a huge step forward, especially for understanding flame-propagation versus autoignition combustion modes."
- "We need to be able to compare results using different strategies in the same engine platform."
- "Optical data leading to conceptual models would be instrumental to advance NG strategies."



Common-platform optical engine can provide the missing science base for multiple NG strategies in reciprocating HD engines

References

1. Figer G, Seitz HF, Graf G, Schreier H "Commercial vehicle natural gas engines with diesel efficiency" MTZ Worldwide 75(10):1-15 (2014)
2. Cornwell R, Foster D, Noble A, "Natural Gas and Dual Fuel Engine Technologies for HDV" IMechE Seminar S1807, London (2014)
3. Smith JR, Green RM, Westbrook CK, Pitz WJ "An experimental and modeling study of engine knock" Proc. Combust. Inst. 20:91-100 (1984)
4. Kokjohn SL "Reactivity controlled compression ignition (RCCI) combustion" Ph.D. Thesis, U. Wisconsin (2012)
5. Perini F, Zha K, Busch S, Miles P, Reitz RD "Principal component analysis and study of port-induced swirl structures in a light-duty optical diesel engine" SAE Tech. Paper 2015-01-1696 (2015)
6. Miles P, Megerle M, Hammer J, Nagel Z, Reitz RD, Sick V "Late-cycle turbulence generation in swirl-supported, direct-injection diesel engines" SAE Tech. Paper 2002-01-0891(2002)
7. Musculus MPB, Lachaux T, Pickett LM, Idicheria CA "End-of-injection over-mixing and unburned hydrocarbon emissions in low-temperature-combustion diesel engines" SAE Tech. Paper 2007-01-0907, SAE Trans. 116(3):515-541 (2007)