Part 7: Diesel combustion and SI knock modeling

Reciprocating Internal Combustion Engines

Prof. Rolf D. Reitz
Engine Research Center
University of Wisconsin-Madison

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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

Diesel engine applications

On-Highway Vehicles

Marine – Propulsion or auxiliary

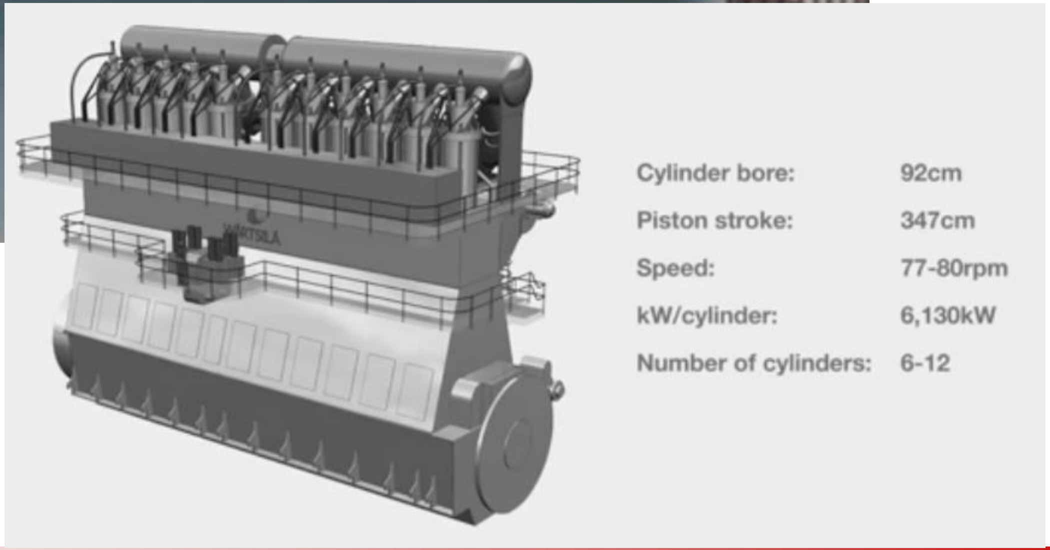
Power Generation – Prime power for remote locations, or standby power for edifices

Locomotive – Switchyard engines, passenger engines, European light freight

Off-Highway Vehicles – Mine trucks (haulers, loaders, etc)

Off-Highway Stationary – Petroleum industry (drill rigs, pumps, etc.)

Diesel engine applications



Cylinder bore:	92cm
Piston stroke:	347cm
Speed:	77-80rpm
kW/cylinder:	6,130kW
Number of cylinders:	6-12

http://maniacworld.com/Worlds-Most-Powerful-Diesel-Engine.html

Diesel combustion

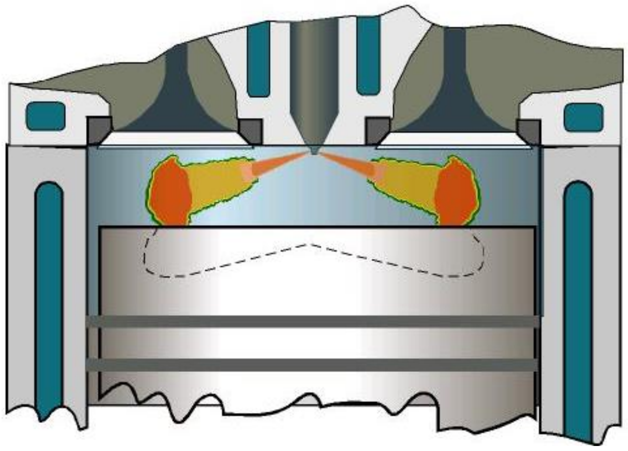
Air alone is drawn in and compressed

Fuel injected into high temperature, high pressure air to initiate combustion

Load controlled by quantity of fuel injected

Highly heterogeneous mixture in cylinder

- wide range of mixture concentration over which combustion occurs
- wide range of operating air-fuel ratios

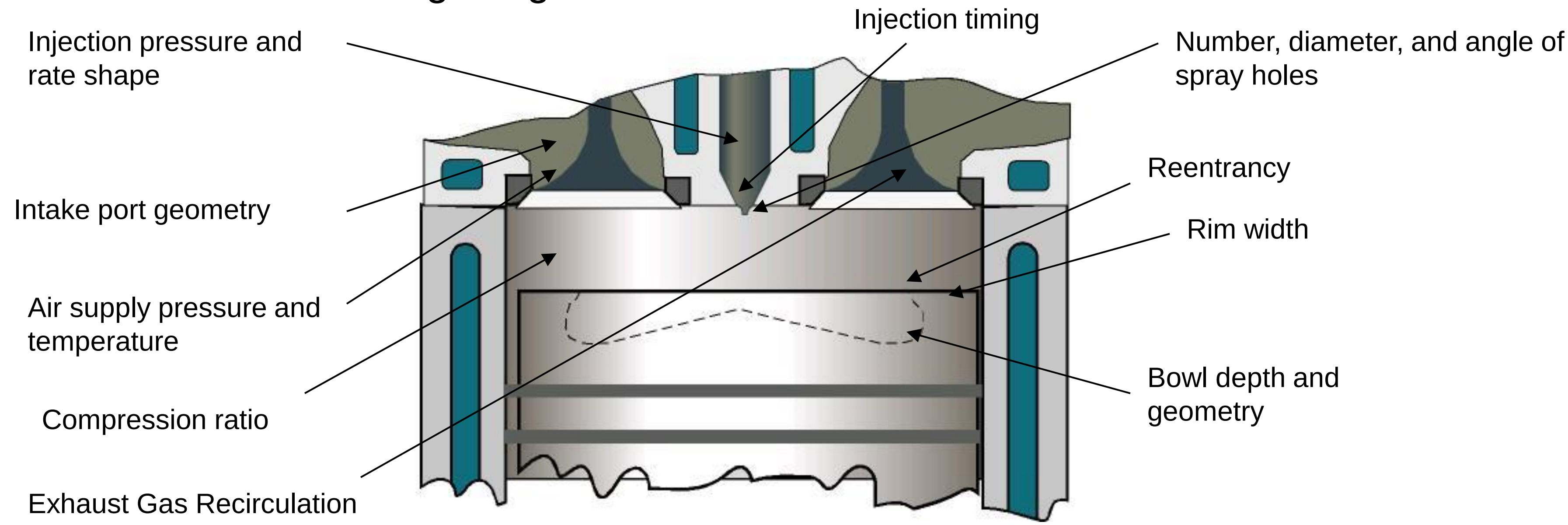


Parameter	Quiescent	Medium Swirl	High Swirl
Cylinder Size	Largest	Medium	Smallest
Maximum Speed (rpm)	100–1800	1800–3000	3000–5000
Range of Bore (mm, inches)	900–150 mm	150–100 mm	130–80 mm
Compression Ratio	12–15	15–16	16–18
Combustion Chamber	Shallow Bowl	Moderate Bowl	Deep Bowl
Injection Pressure	Highest	High	Moderate
Number of nozzle holes	Multiple	Multiple	Multiple
In-Cylinder Air Flow	Quiescent	Medium Swirl	High Swirl

Diesel combustion - General Rules

Center fuel injector in bowl, and if possible, center bowl in piston

Trade off fuel injection pressure versus air motion to provide required mixing while not over-mixing at light load

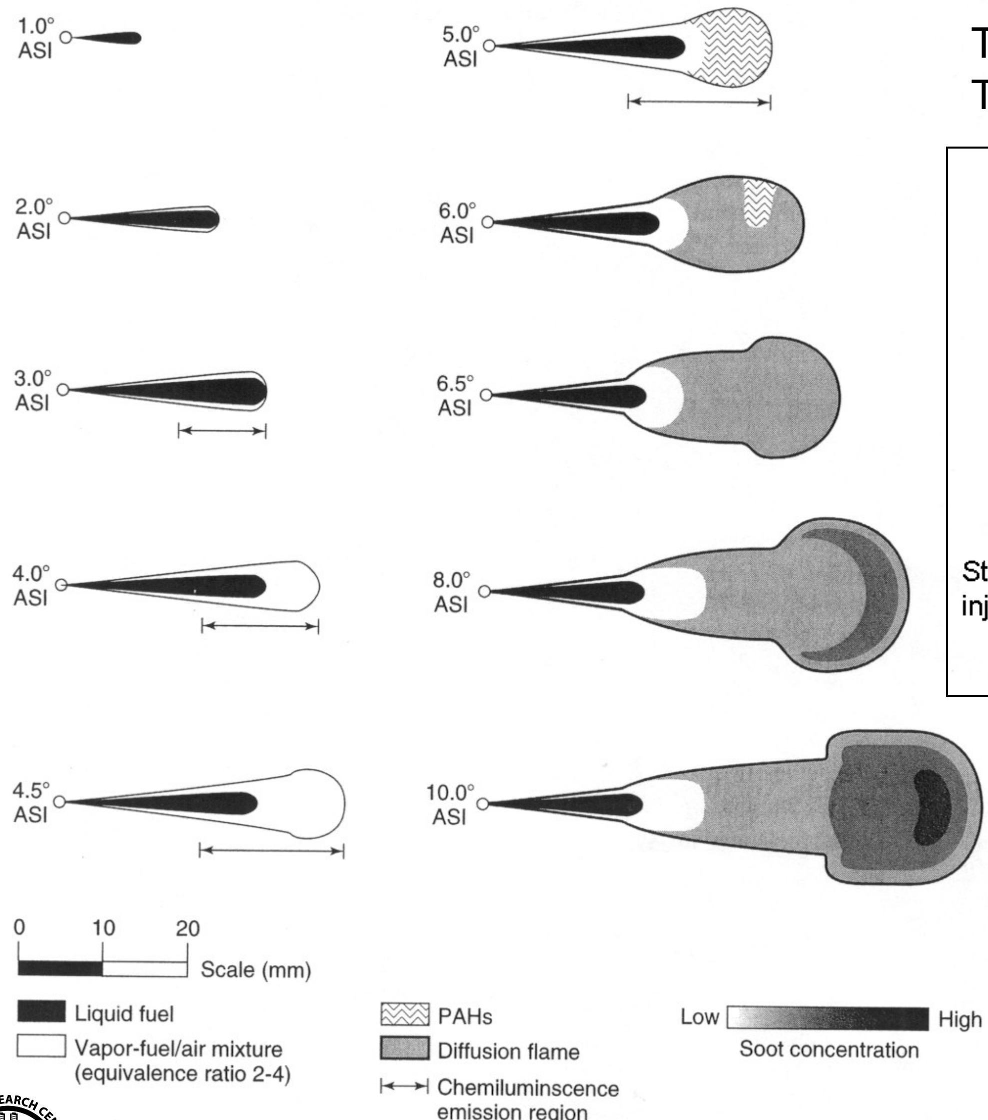


Supply sufficient air to meet peak torque smoke limits

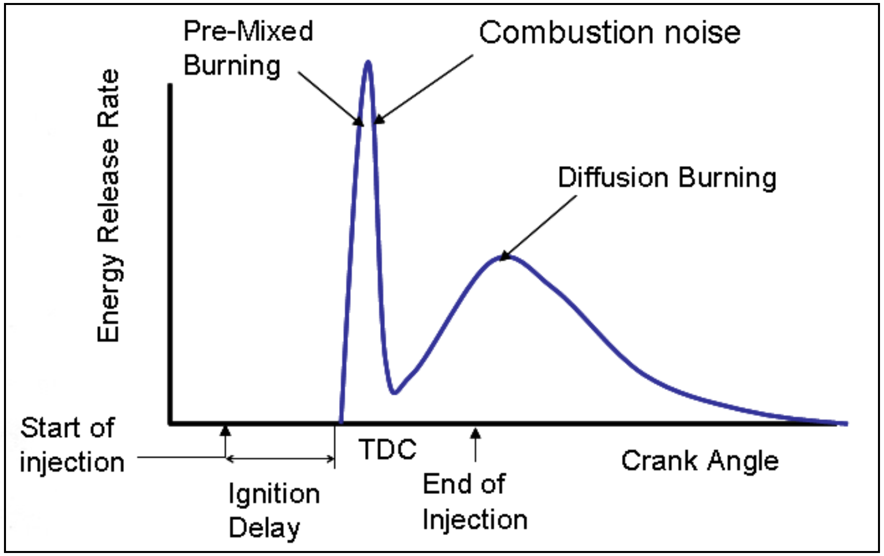
Select injection timing and compression ratio for best fuel economy within emission constraints

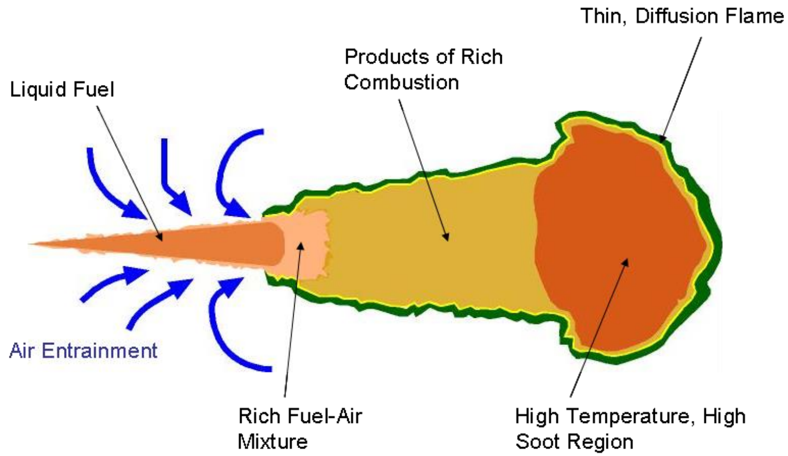
Other constraints: peak cylinder pressure, fuel injection pressure

Diesel combustion (Conceptual model of Dec, 1997)



Time to mix fuel/air to “combustible” ratios
Time at given T and P to initiate combustion

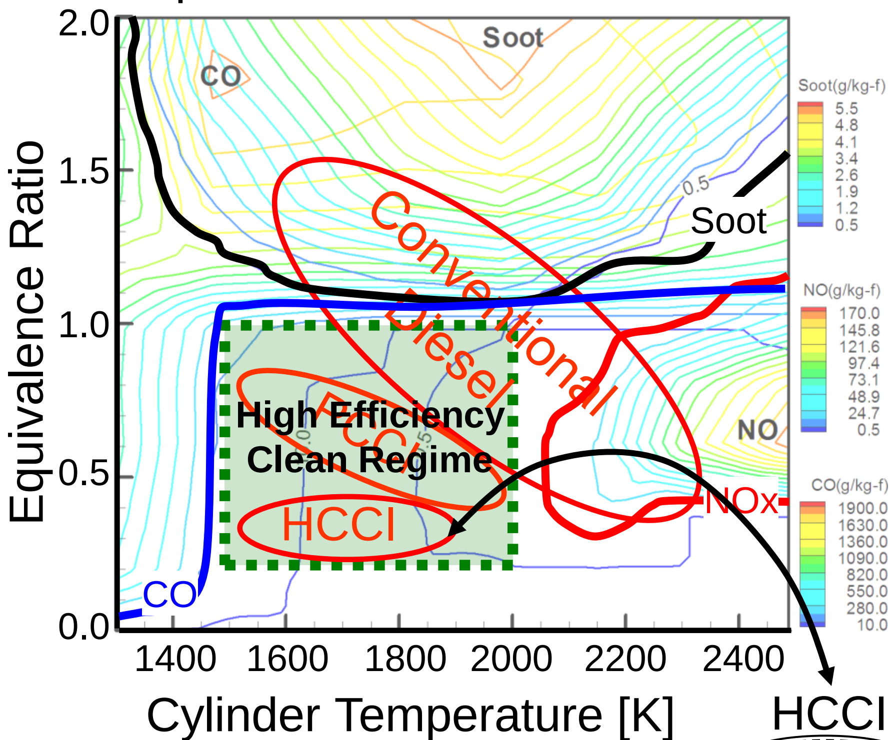


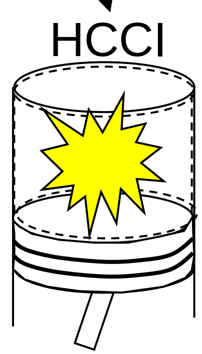


Park, 2007

Diesel combustion regimes

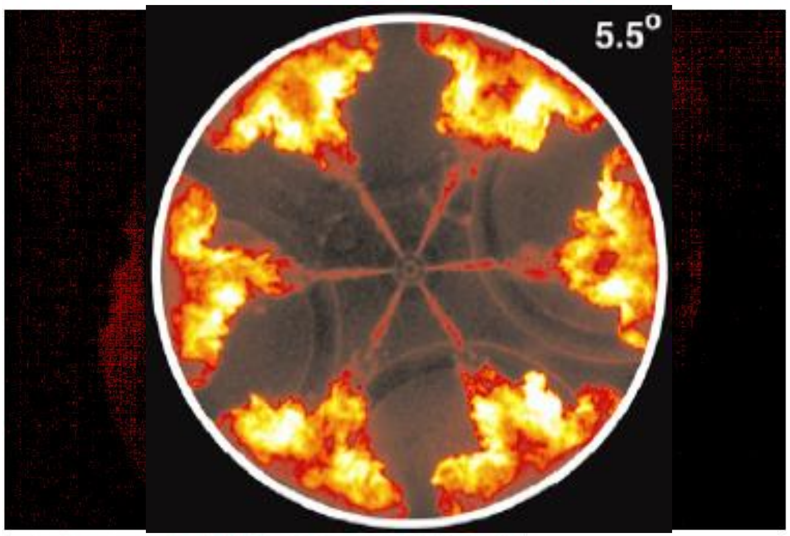
Kamimoto plot



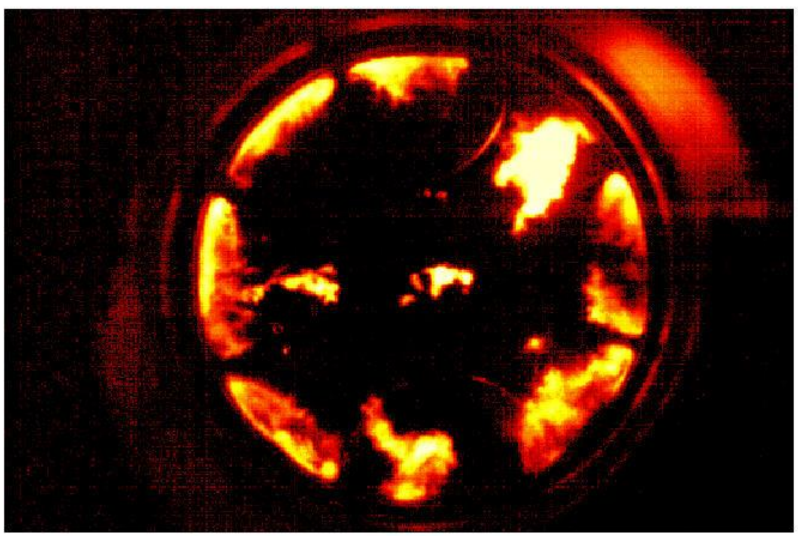


Requires precise charge preparation and combustion control mechanisms (for auto-ignition and combustion timing)

Conventional diesel



Early injection PCCI



Musculus 2006

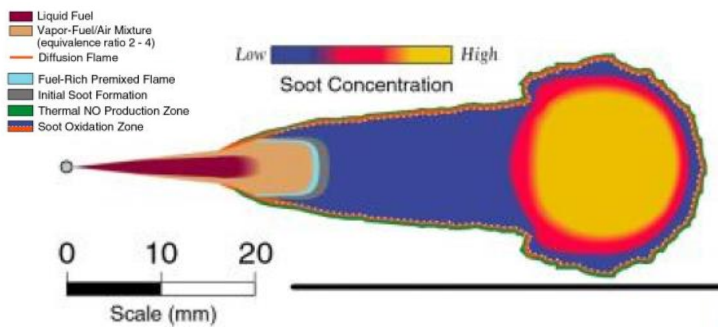
Dec, 1997

Diesel combustion regimes

Conventional Diesel

Dec used optical diagnostics to develop a conceptual model of conventional diesel combustion

OH exists only at periphery of the jet → thin diffusion flame surrounding a soot filled jet



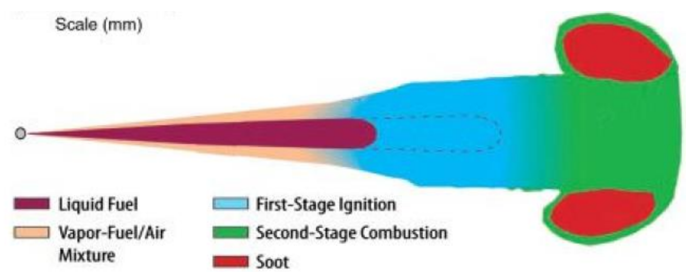
Dec's conceptual model

LTC diesel Combustion

Musculus developed a similar conceptual model for diesel LTC

Low temperature reactions fill the head of the jet with intermediates (e.g., CH_2O)

OH is observed across the entire jet cross-section



LTC conceptual model

Diesel combustion modeling

KIVA-CHEMKIN-G code

CHEMKIN II based chemistry solver used for volumetric heat release

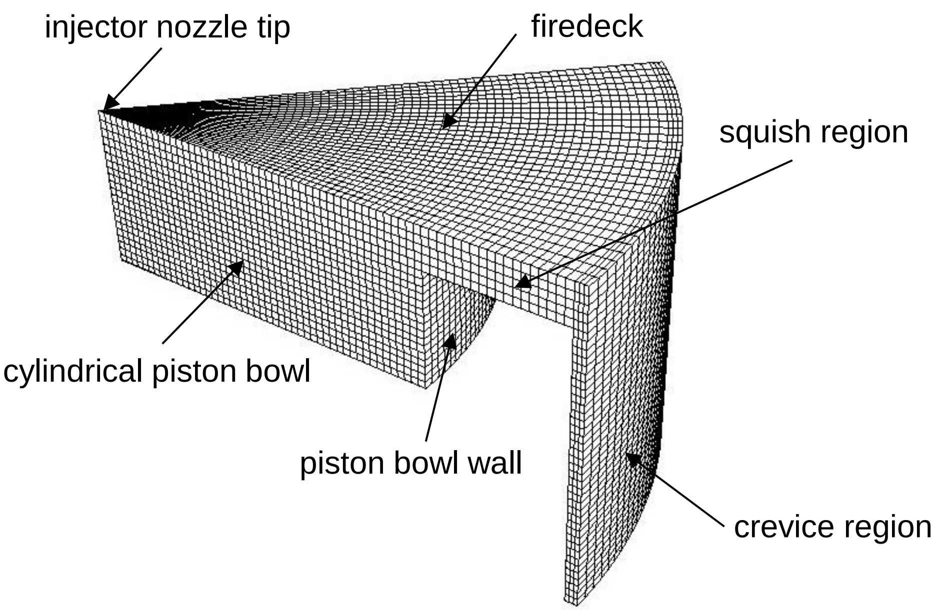
- Each cell considered a well-stirred reactor (WSR)
- Diesel fuel chemistry is modeled with ERC reduced n-heptane mechanism

Flame propagation considered through level set based model → G equation

Spray modeled with ERC spray models

- Gasjet theory used to reduce grid size dependency of droplet drag calculations
- Collision model considers bounce, coalescence, and fragmenting and non-fragmenting separations
- KH-RT breakup model

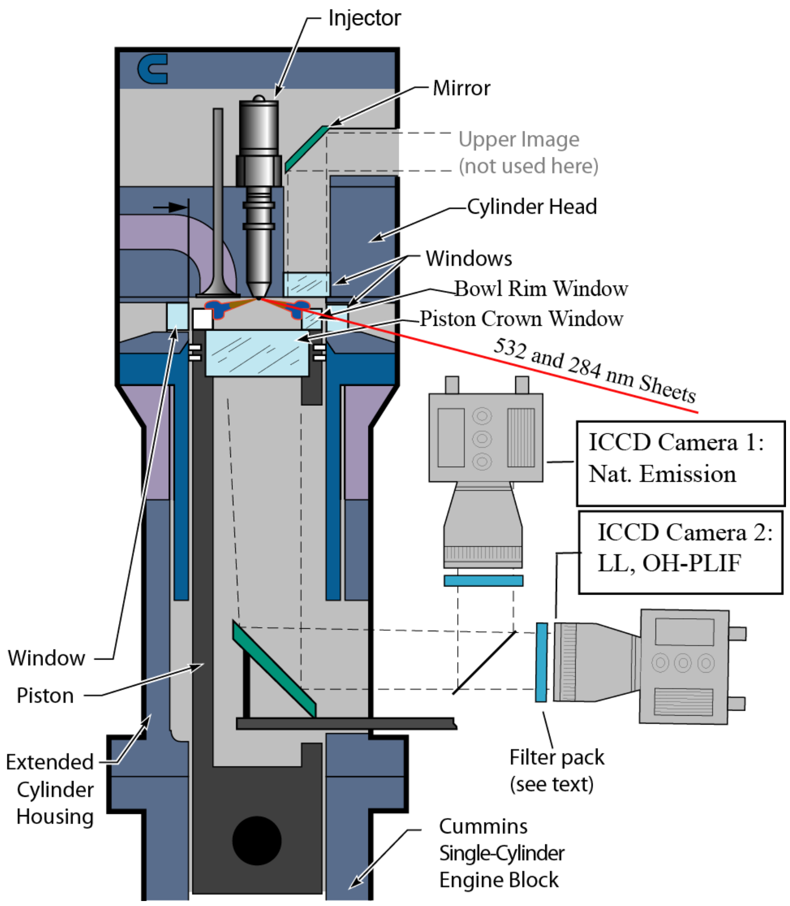
Tetradecane used for fuel physical properties



Singh, 2009

Engine setup – Sandia Cummins

Base engine type	Cummins N-14 DI diesel
Number of cylinders	1
Bore x stroke	13.97 x 15.24 cm
Connecting rod length	30.48 cm
Displacement	2.34 L
Geometric compression ratio	10.75:1
Simulated compression ratio	16:1
Bowl width	9.78 cm
Bowl depth	1.55 cm
Fuel injector type	Common-rail
Cup (tip) type	mini-sac
Number of holes	8, equally spaced
Spray included angle	152°
Nozzle orifice diameter	0.196 mm
Nozzle orifice L/D	5



Singh, 2009

Operating conditions

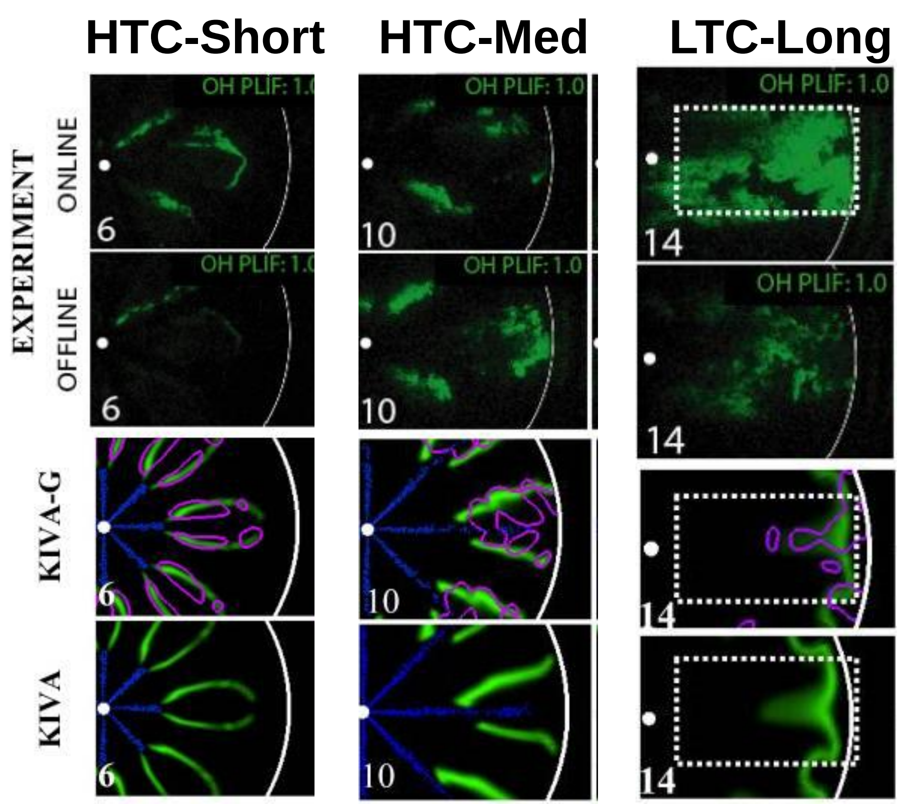
Three cases ranging from Conventional to LTC diesel combustion

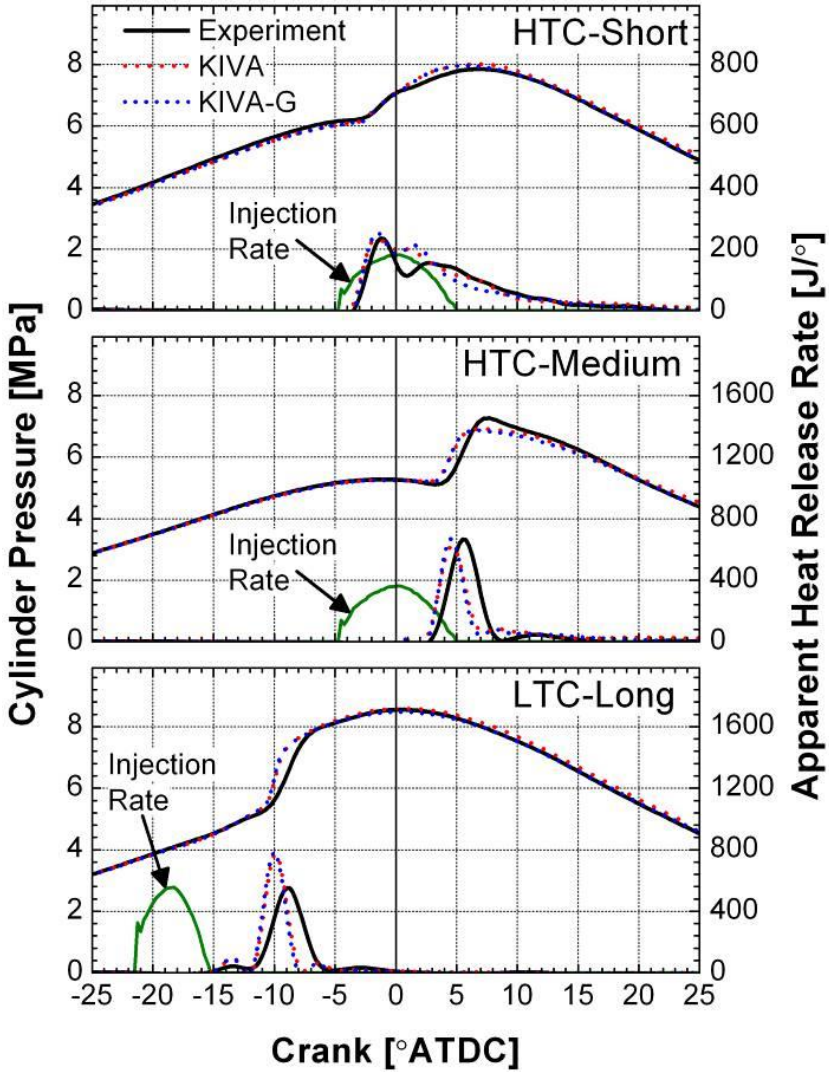
	HTC- short ID	HTC- med. ID	LTC- Long ID
O_2 Conc. (Vol %)	21	21	12.7
Speed (RPM)	1200	1200	1200
IMEP (bar)	4.5	4.5	3.9
Intake Temp (°C)	111	47	90
Intake Pressure (kPa)	233	192	214
TDC Motored Temperature (K)	905	800	870
TDC Motored Density (kg/m3)	24	22.3	22.9
Peak Adiabatic Flame Temp. [K]	2760	2700	2256
Rail Pressure (bar)	1200	1200	1600
Start of Injection (°ATDC)	-7	-5	-22
Duration of Injection (°CA)	10	10	7
Injection Quantity (mg)	61	61	56
Ignition Delay (°CA)	4	8.75	11
Ignition Dwell (°CA)	-6	-1.25	+4

Kokjohn, 2011

Combustion characteristics

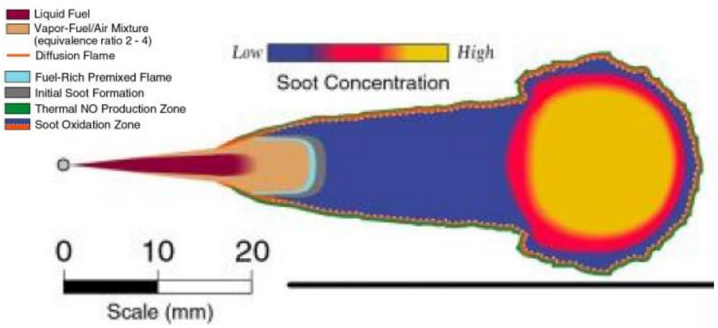
- Simulations capture combustion characteristics accurately over a range of combustion regimes
- Results with and without consideration of flame propagation show nearly identical results





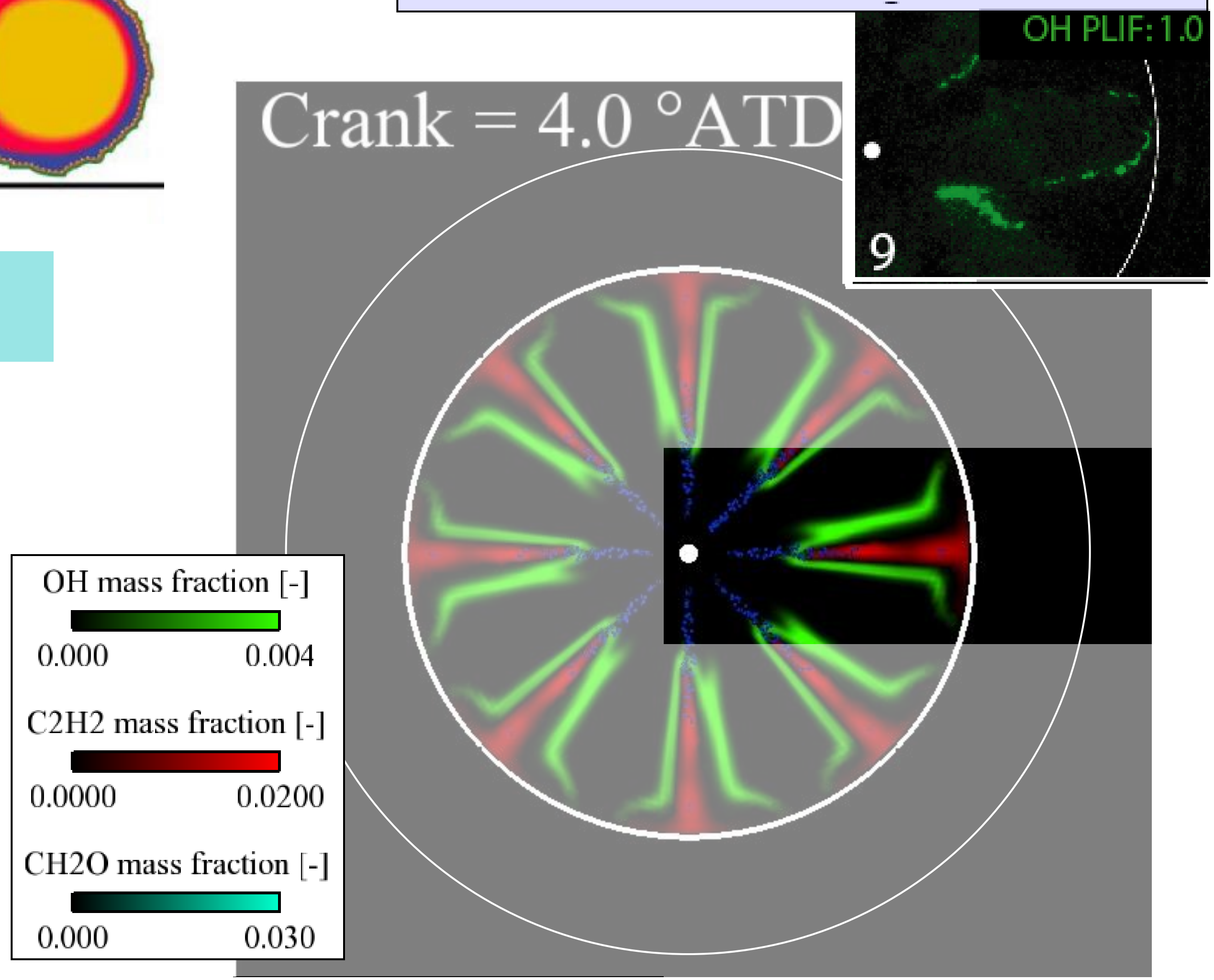
Kokjohn, 2011

Conventional diesel combustion



Dec's conceptual model
SAE 970873

Simulations and experiments show diffusion flame is 1 to 2 mm thick



O2	21%
SOI1	-7 °ATDC
P_{inj}	1200 bar
Intake P	2.33 bar
Fuel	Diesel

Optical engine experiments
Singh, CNF 2009

Kokjohn, 2011

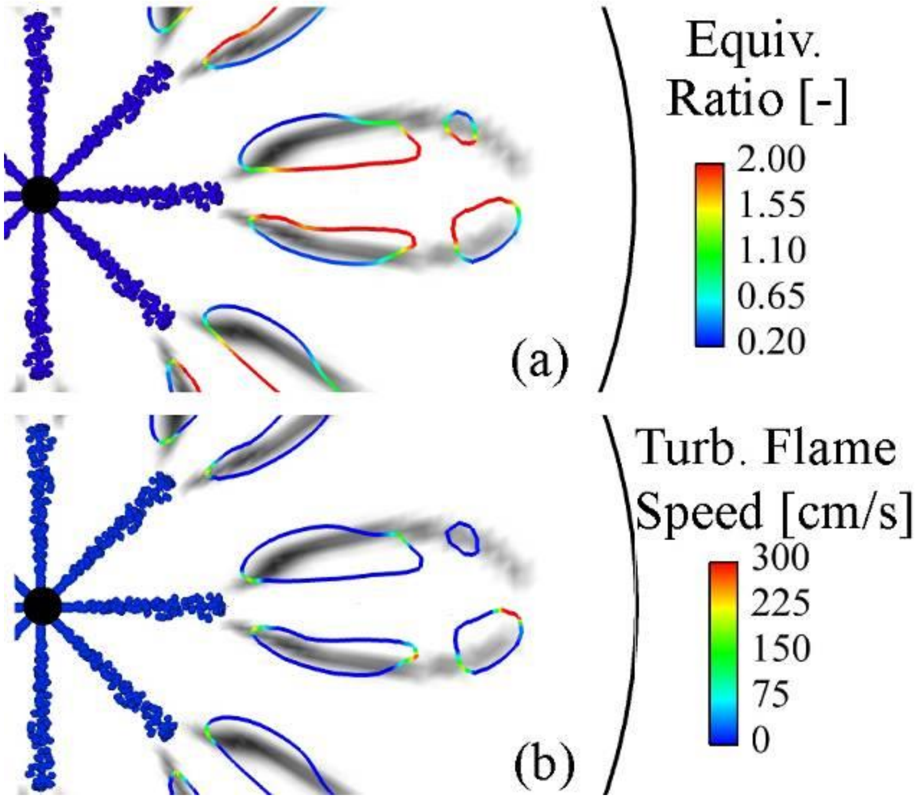
Conventional diesel combustion

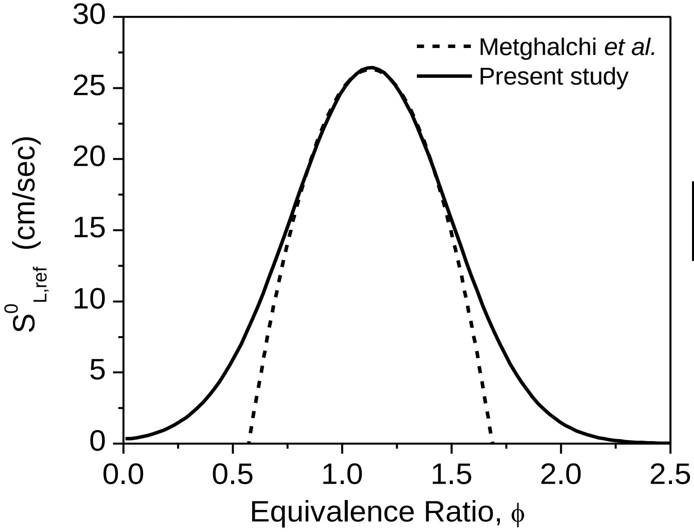
Role of flame propagation:

Flame propagation model predicts edge or triple flame structure near lift-off location

Nose like structure with stoichiometric region closest to nozzle

Stoichiometric region shows the only non-negligible flame speed



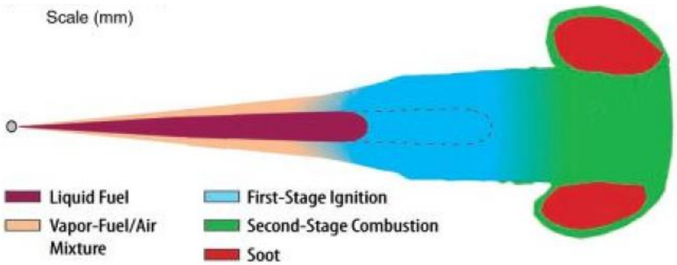


$S_T \sim S_L$

$$\frac{\partial \tilde{G}}{\partial t} + (\vec{v}_f - \vec{v}_{vertex}) \cdot \nabla \tilde{G} = \frac{\bar{\rho}_u}{\bar{\rho}} S_T^0 \left|\nabla \tilde{G}\right| - D_T \tilde{k} \left|\nabla \tilde{G}\right|$$

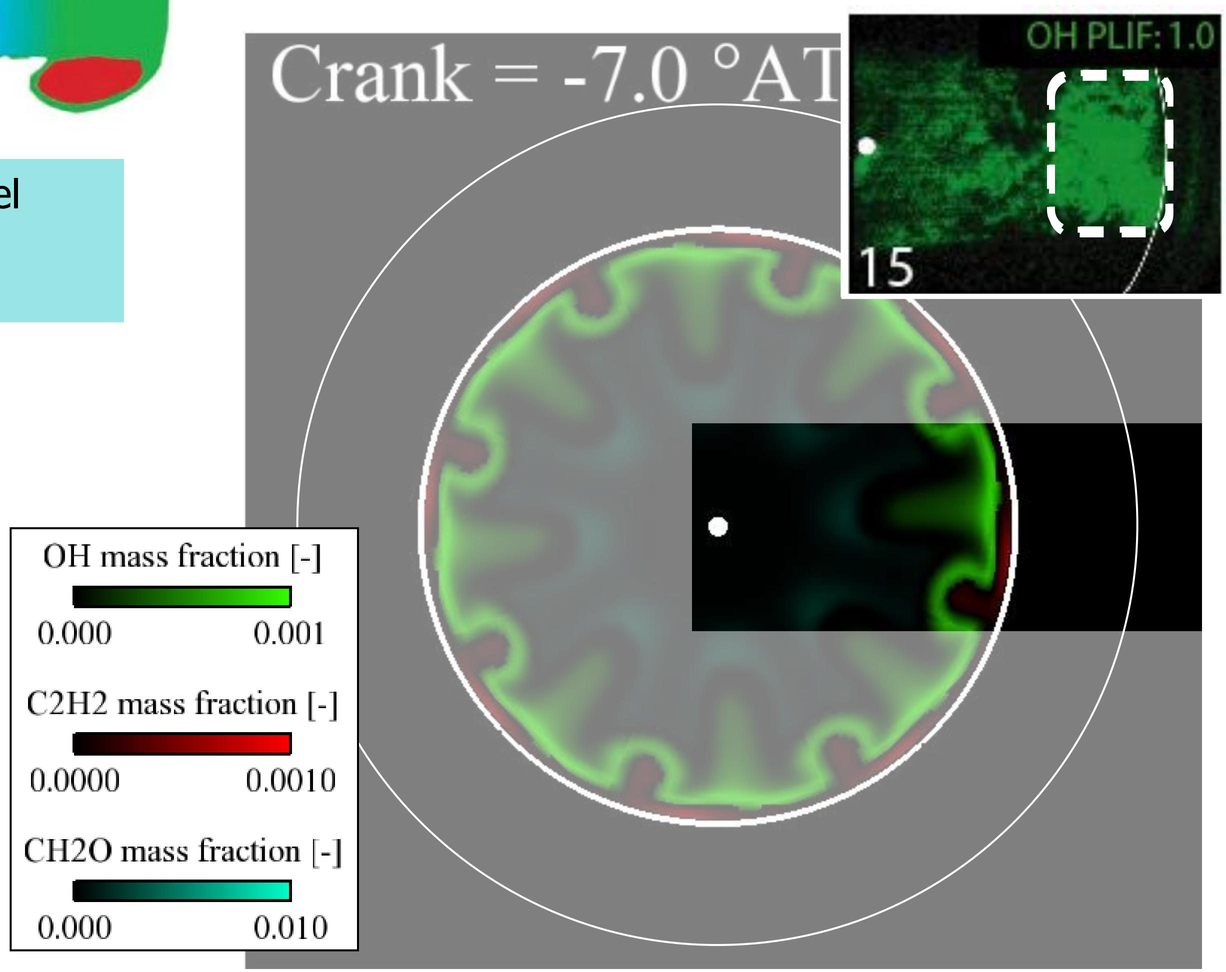
Kokjohn, 2011

LTC diesel combustion



LTC conceptual model
Musculus et al.
SAE 2006-01-0079

Increased mixing time allows OH to fill jet



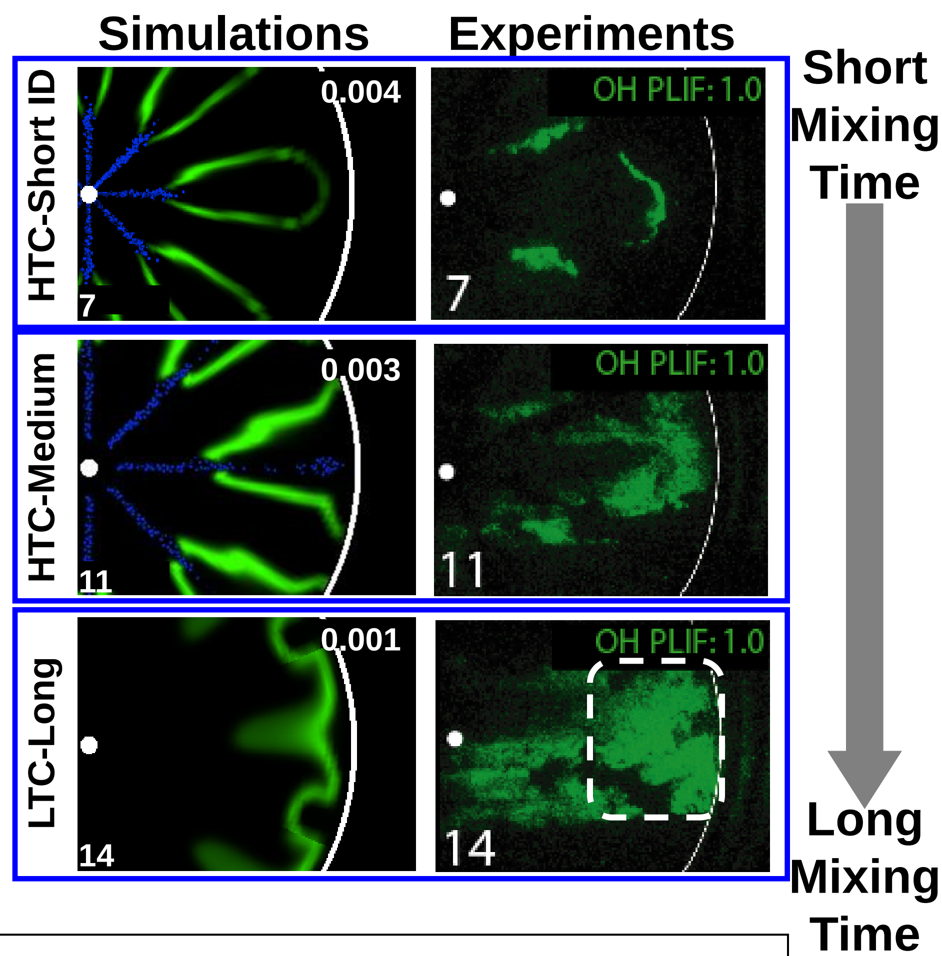
O2	12.7%
SOI1	-22 °ATDC
P_{inj}	1600 bar
Intake P	1.92 bar
Fuel	Diesel

Optical engine experiments
Singh, CNF 2009

Kokjohn, 2011

Dependence of flame structure on mixing time

- HTC – Short ID
  - Diffusion flame is 1-2 mm thick
- HTC – Medium ID
  - Diffusion flame is 4 – 6 mm (exp. show 5 – 6 mm)
- LTC – Early (Long ID)
  - OH fills jet
- Increase in reaction zone thickness with mixing time



- Flame structure is captured **without** considering sub-grid scale turbulent/chemistry interactions
- Ignition occurs in premixed region

- Combustion is controlled by diffusion and large scale (resolved) mixing processes

Reaction rate dependence on injection-generated mixing decreases with increasing ignition delay. If ID extends past end-of-injection, combustion-generated-mixing dominates injection-generated-mixing

Kokjohn, 2011

Singh, 2009

Flame thickness dependence on equivalence ratio

Singh et al. (2009) studied dependence of equivalence ratio on OH LIF using homogenous reactor and 1D opposed flow diffusion flame simulations

HTC-Short ID (21% O2)

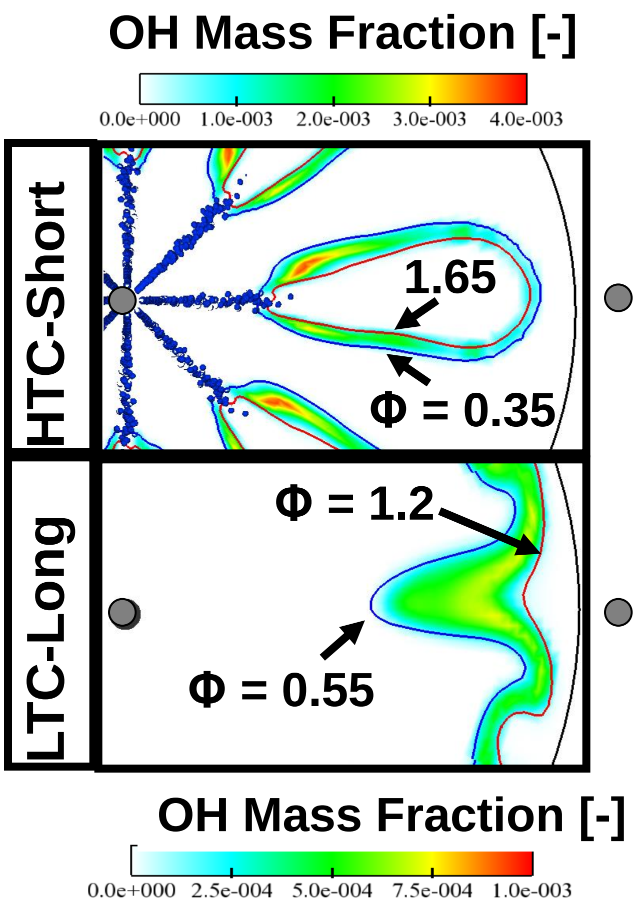
OH detectable when 0.2 < Φ < 1.6

LTC-Long ID (12.7% O2)

OH detectable when 0.5 < Φ < 1.2

Kokjohn & Reitz (2011) CFD simulations show similar dependence on equivalence ratio

For a given intake oxygen concentration, OH LIF can be used to estimate local equivalence ratios



Reaction zone thickness and equivalence ratio are correlated.

Kokjohn, 2011

Relative importance of turbulence and chemistry

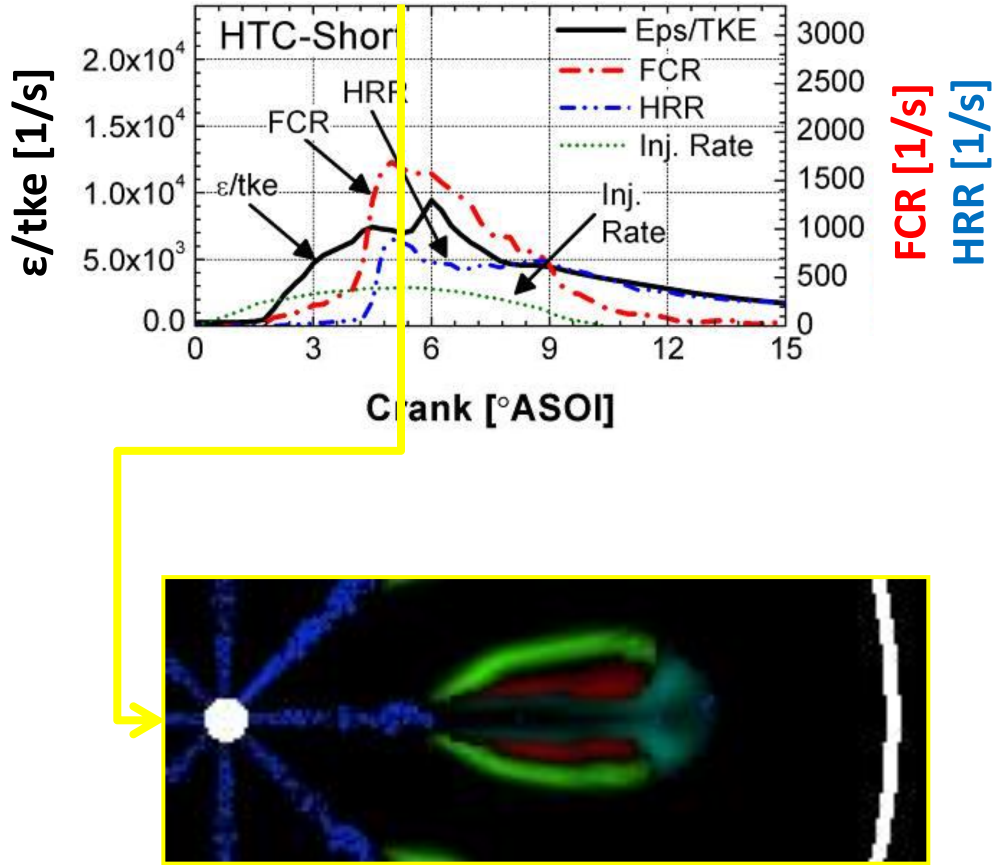
HTC-Short ID

Initial reactions occur in a well mixed zone on the periphery of the jet (Φ~1)

Kinetically controlled premixed spike followed by a mixing controlled energy release

Turbulent mixing due to the injection event remains elevated during energy release

Reaction rate is controlled by the rate of transport of reactive material to the reaction zone



Kokjohn, 2011

Relative importance of turbulence and chemistry

HTC-Medium ID

Sharp increase in turbulent mixing rate due to injection event

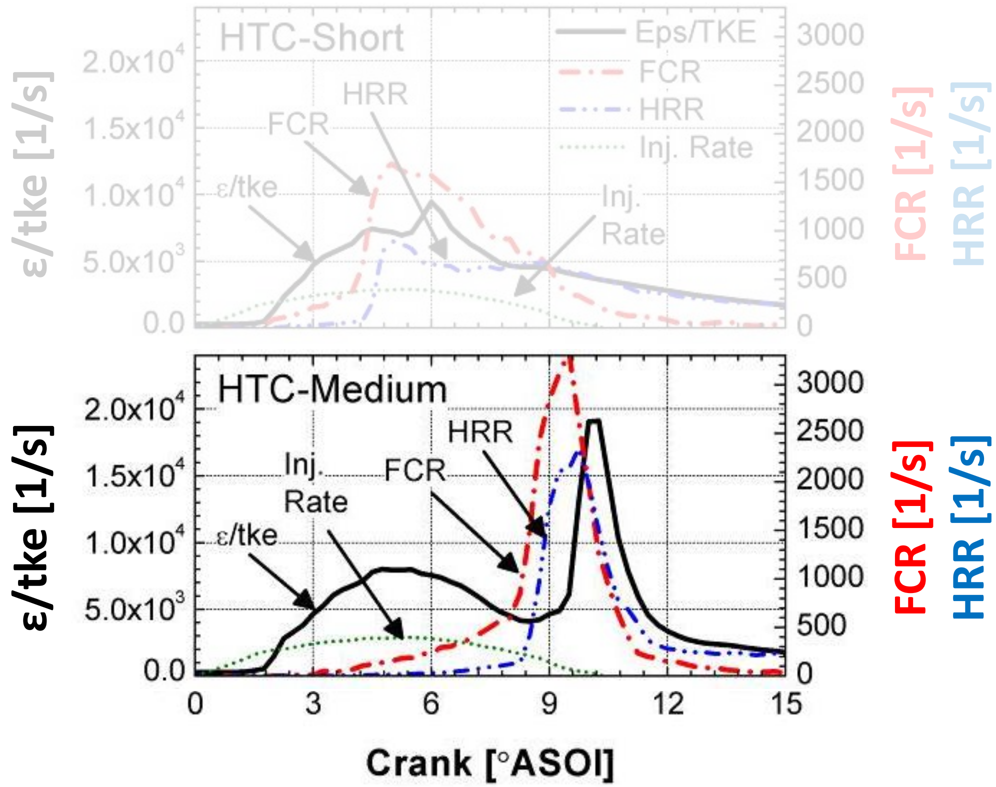
Injection event is nearly complete by SOC

Turbulent mixing rate has started to decrease prior to auto-ignition

Second spike in the mixing rate due to expansion of hot products

Occurs after a significant quantity of the fuel has already been consumed

Spray induced mixing less important as ignition dwell approaches zero



Kokjohn, 2011

Relative importance of turbulence and chemistry

LTC-Long ID

Sharp increase in turbulent mixing rate due to injection event

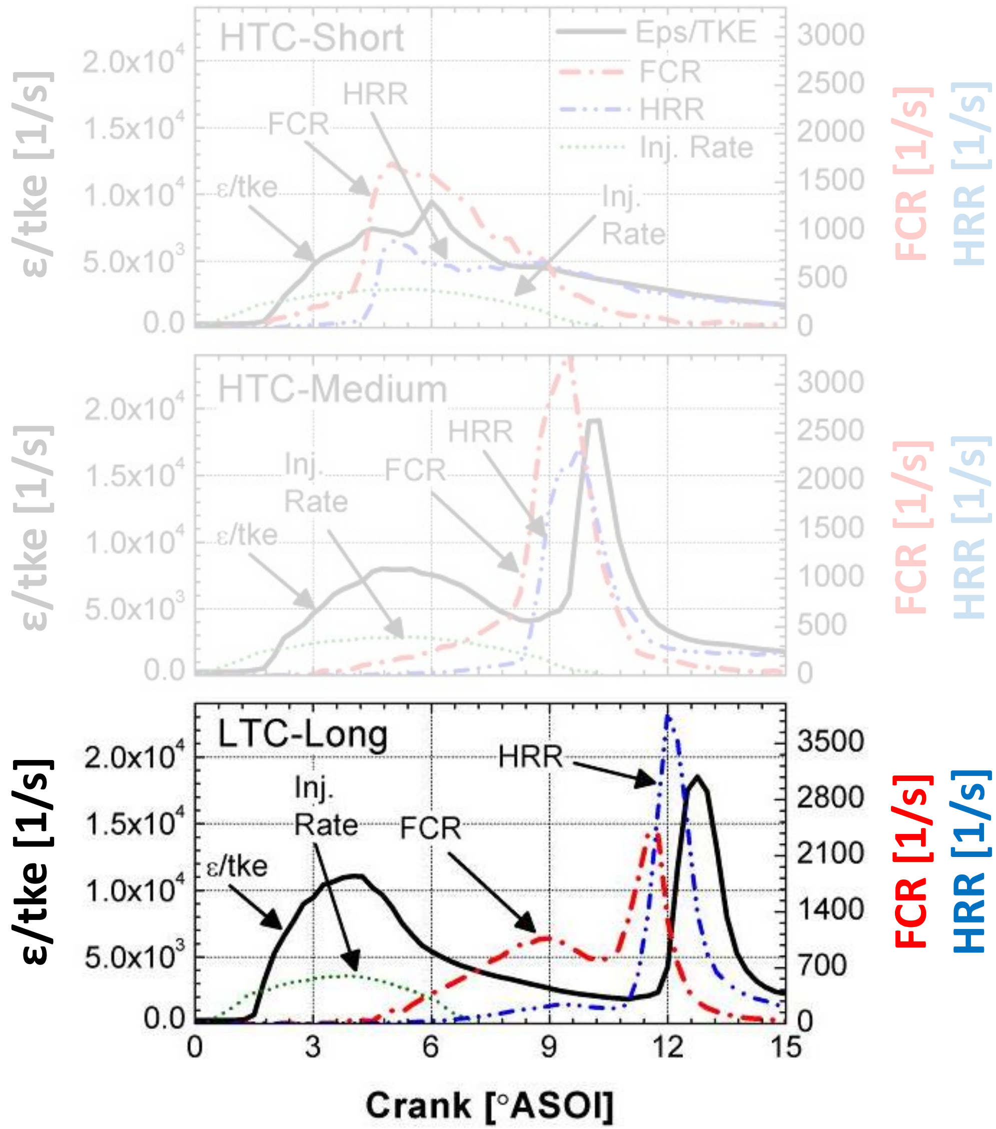
Injection event is completed prior to second-stage combustion

Mixing rate has dissipated nearly completely prior to auto-ignition

Fuel is consumed in two distinct stages

HR occurs rapidly and has nearly completed by the second spike in the mixing rate

Turbulent mixing appears to play a secondary role to kinetics

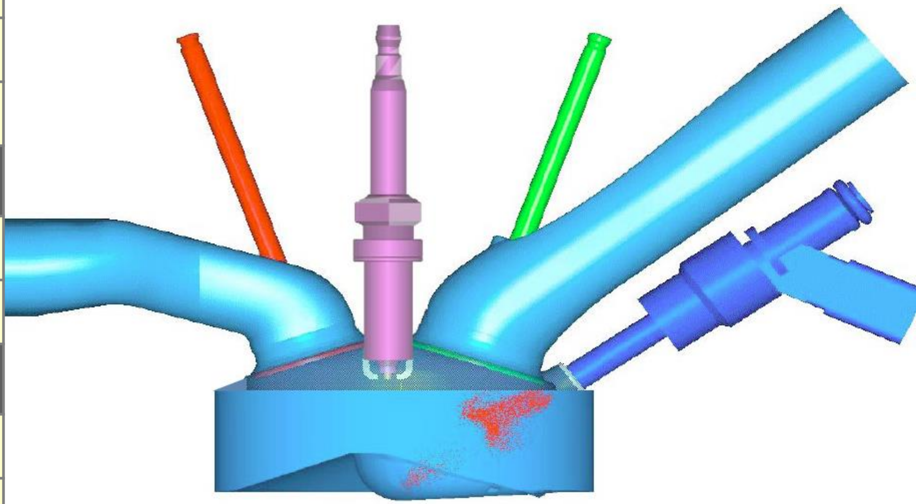


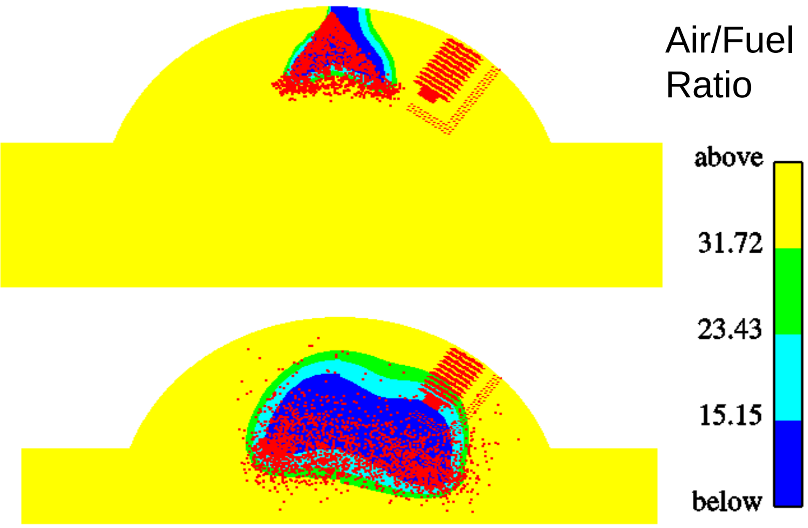
Liang, 2007

Subramaniam, 2003

Spark-ignition gasoline engine knock

Bore × Stroke	89 mm × 79.5 mm
Compression Ratio	12 : 1
Engine Speed	1500 rev/min
PFI Mode	
Spark timings (ATDC)	-44, -40, -36, -32
MAP (kPa)	65
DI Mode (Spark timing sweeps)	
Spark timings (ATDC)	-32, -28, -24, -20
MAP (kPa)	75
End of Injection (ATDC)	- 72
DI Mode (Manifold-Absolute-Pressure sweeps)	
MAP (kPa)	75, 80, 90, 100
Spark timing (ATDC)	- 33
End of Injection (ATDC)	- 68
DI Mode (End-Of-Injection sweeps)	
End of Injection (ATDC)	-76, -72, -68, -64
MAP (kPa)	75
Spark timing (ATDC)	- 32

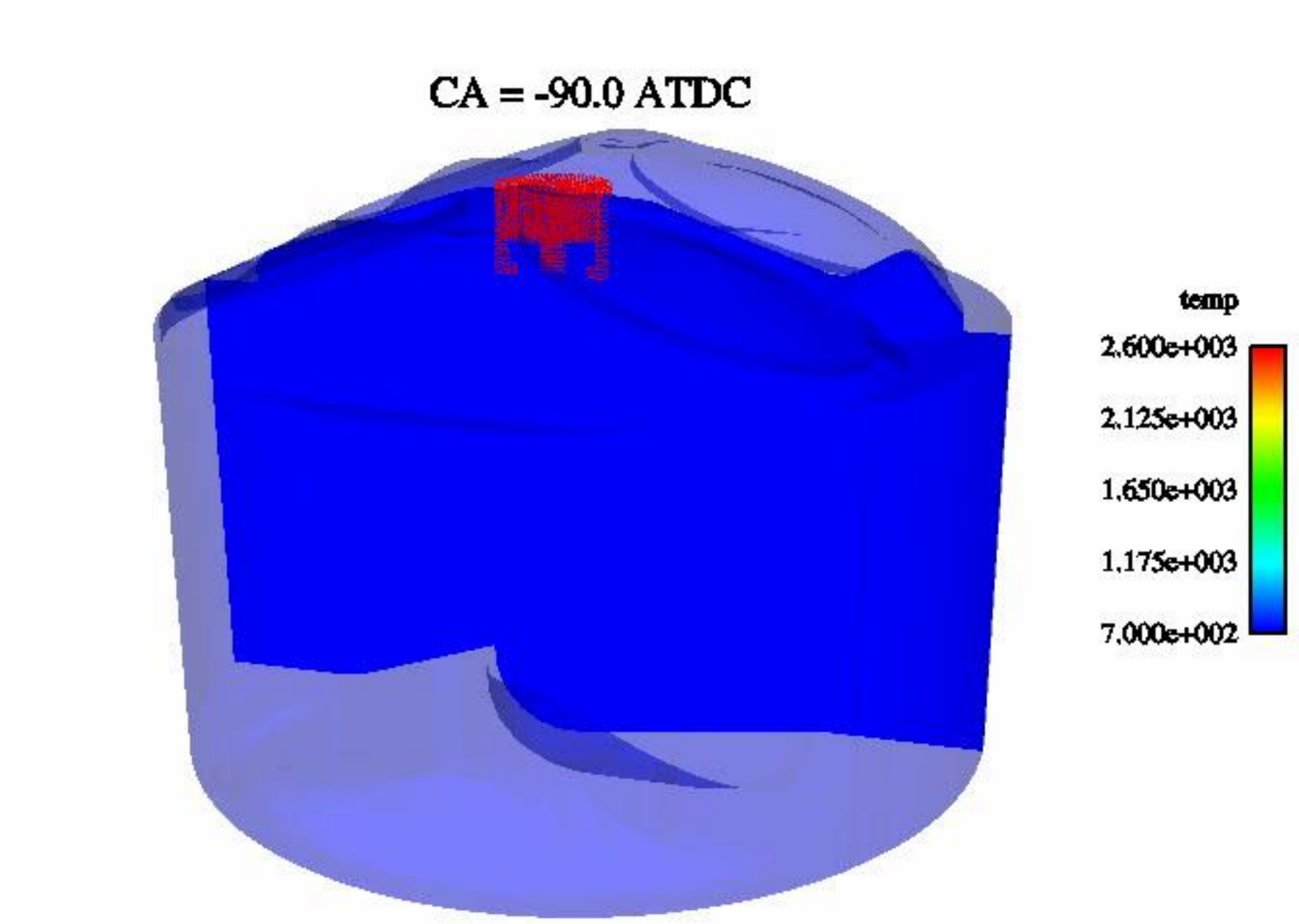




Liang, 2007

Subramaniam, 2003

Direct injection flame propagation



ERC spray models

DPIK ignition model

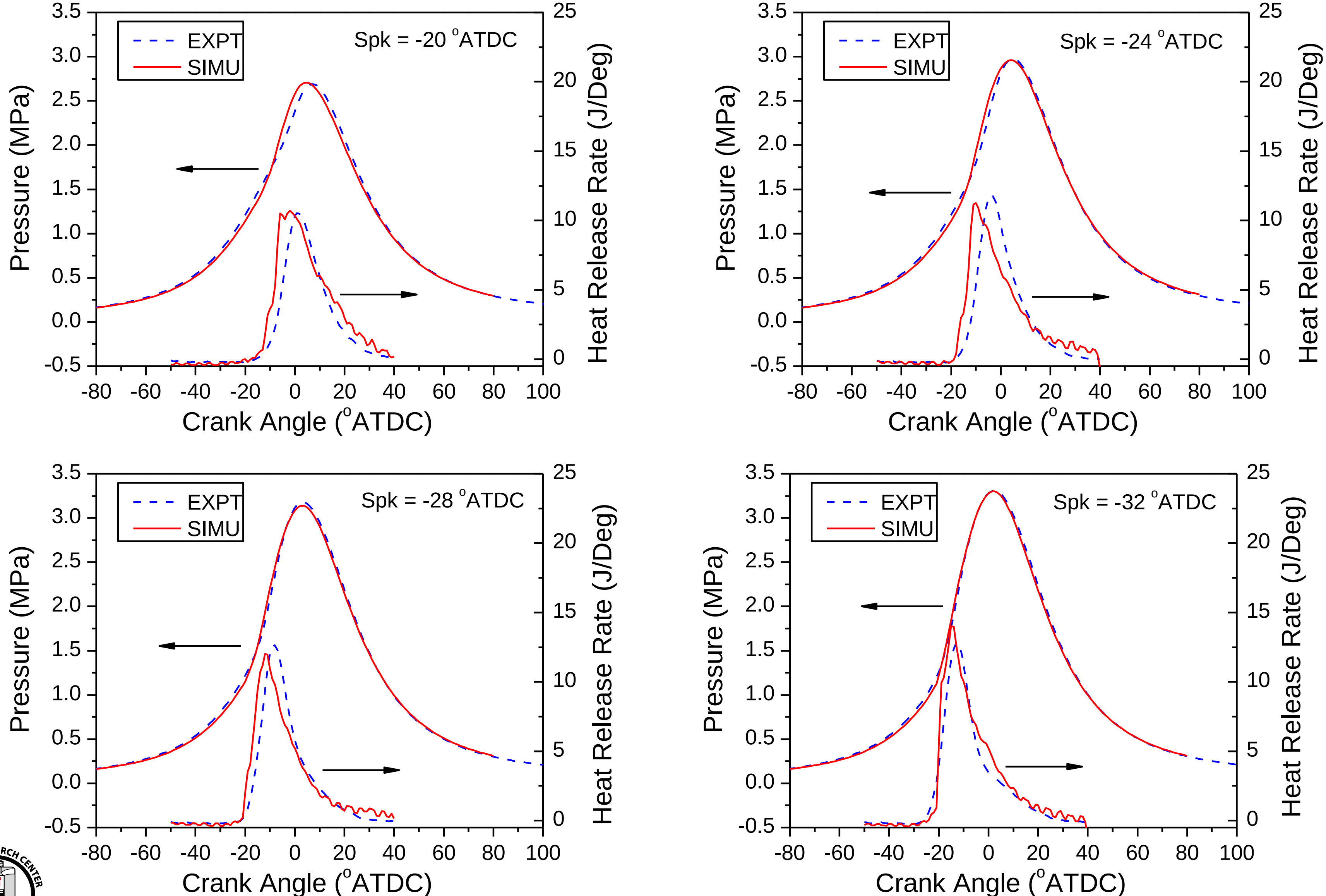
KIVA-Chemkin-G with ERC PRF mechanism

ERC reduced NOx mechanism

Spark Timing = -32 ATDC

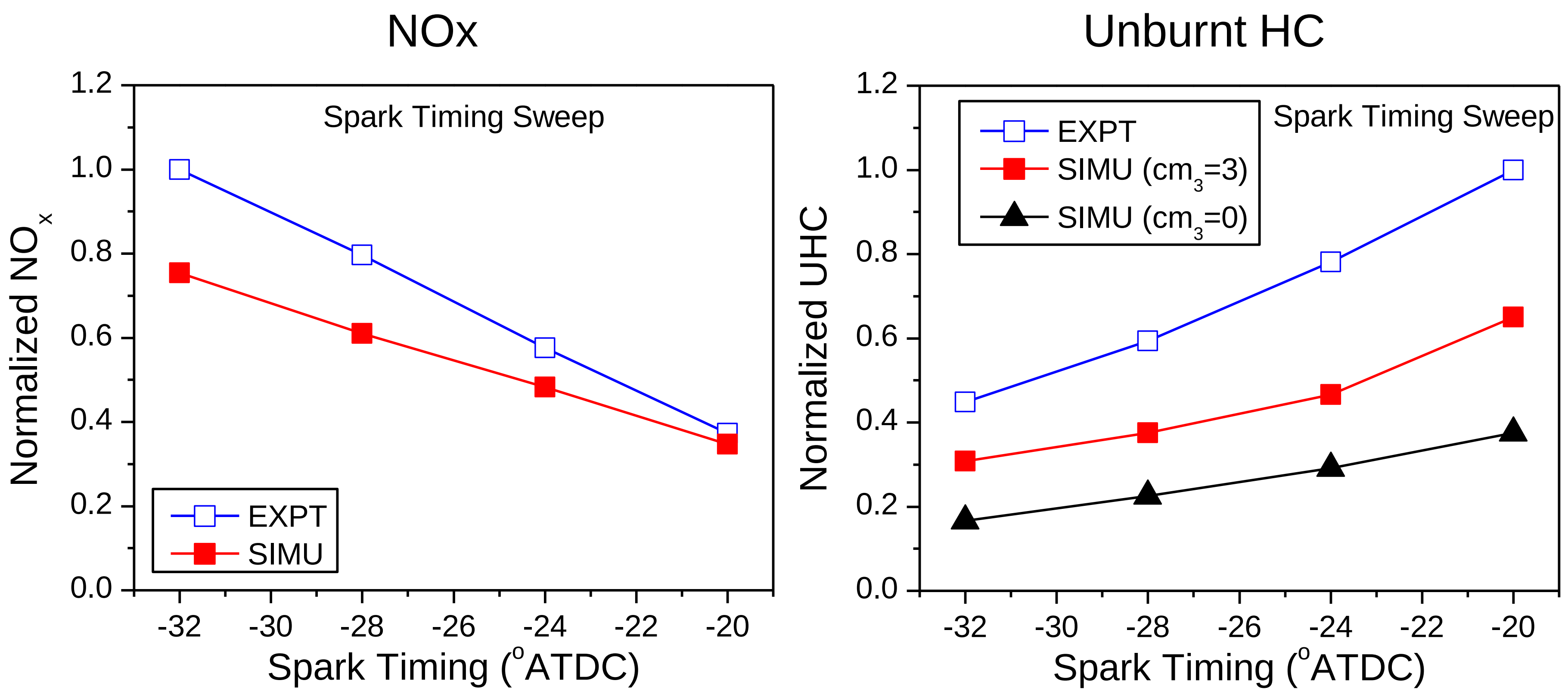
Liang, 2007

Validation - spark timing sweep



Liang, 2007

Validation - Spark Timing Sweep



Local flame quench due to mixture stratification is modeled:

$$l_K < C_{m3} l_\delta = C_{m3} \delta l_F$$

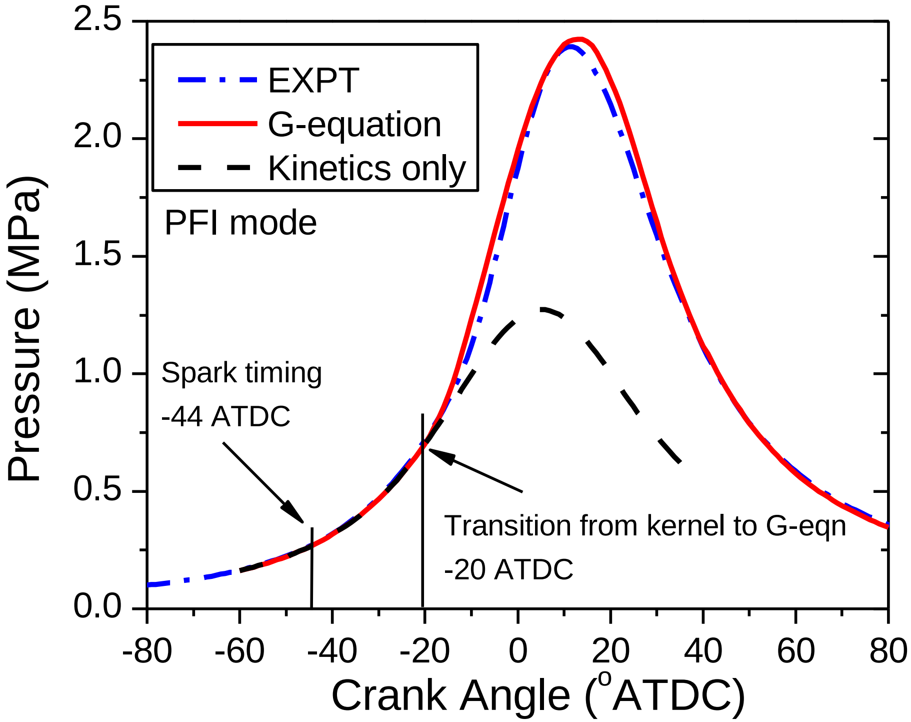
Liang, 2007

Role of turbulence in SI combustion

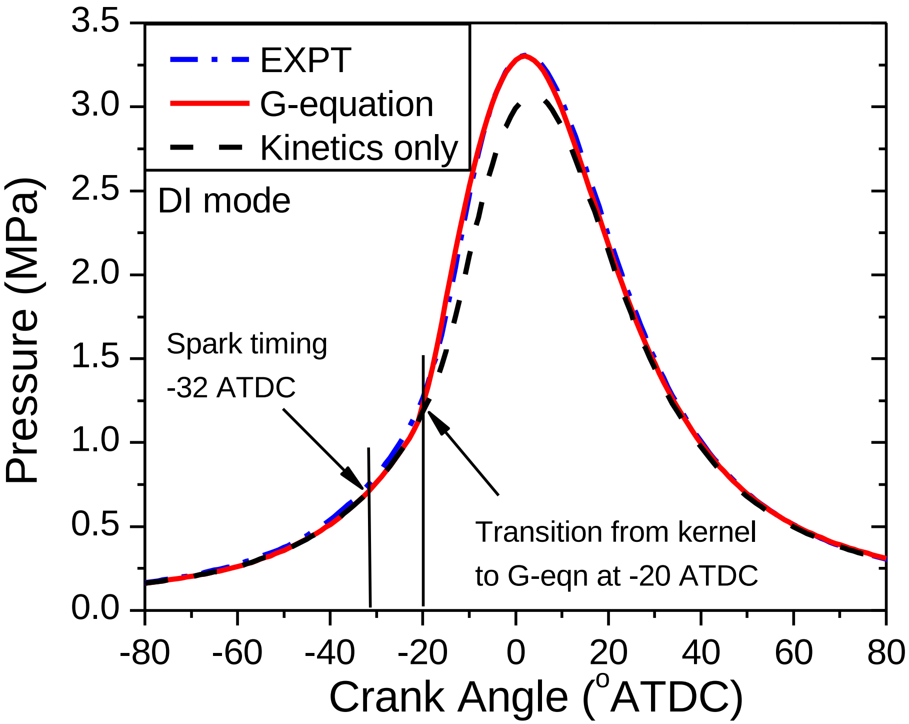
Kinetics-Controlled Formulation for Turbulent Flame Propagation:

After ignition kernel stage, each cell modeled as WSR, & detailed chemistry applied

“Flame propagation” is controlled by heat conduction and auto-ignition instead of G-equation model.



PFI (Spark timing = - 44 ATDC)



DI (Spark timing = - 32 ATDC)

Liang, 2007

Assessment of kinetics-controlled combustion models

PFI case
Spark timing = -44 ATDC

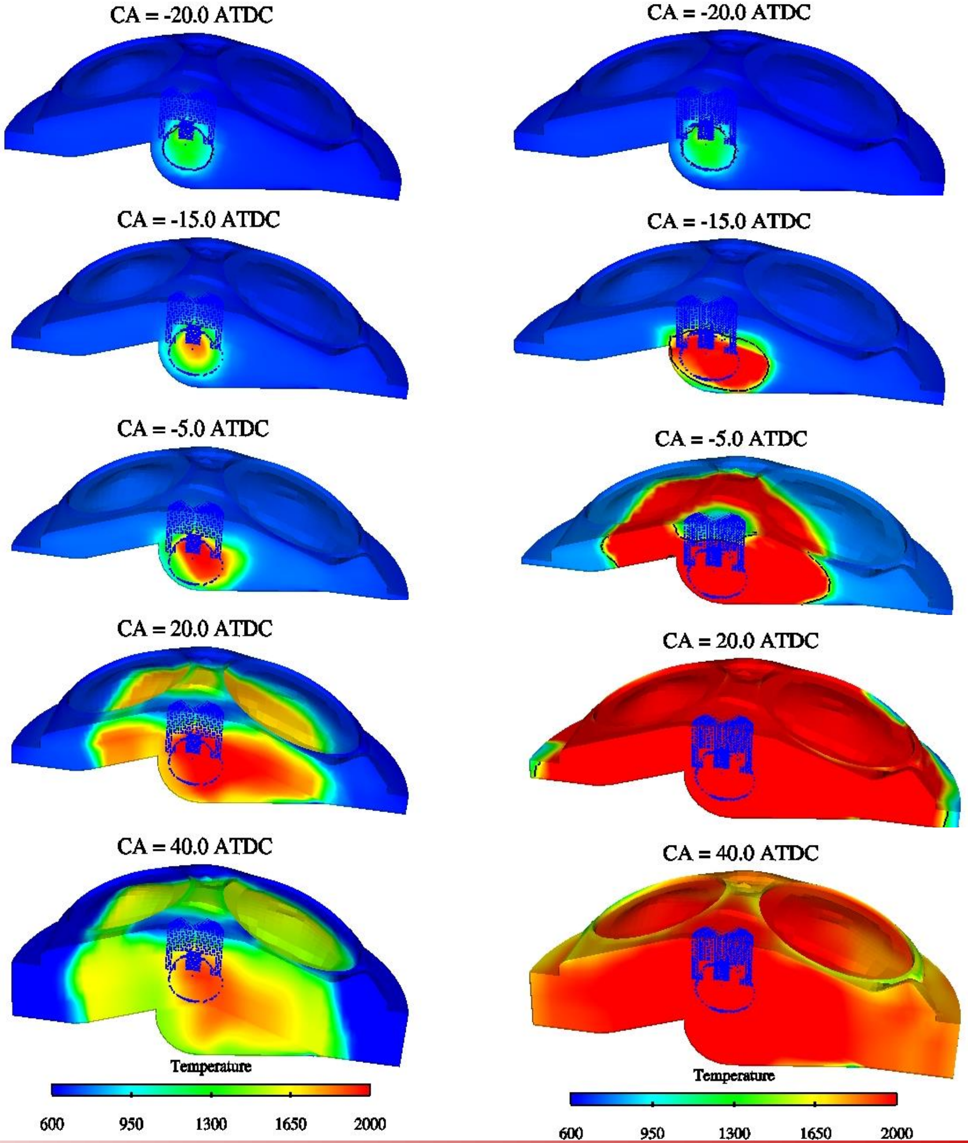
Conclusion:

Auto-ignition chemistry alone is NOT sufficient to properly model flame propagation.

Turbulence enhancing effect on flame propagation speed in premixed charge SI engines CANNOT be neglected.

However, in direct injection cases combustion is controlled by mixing rates (diffusion combustion).

Kinetics Controlled | *G*-equation



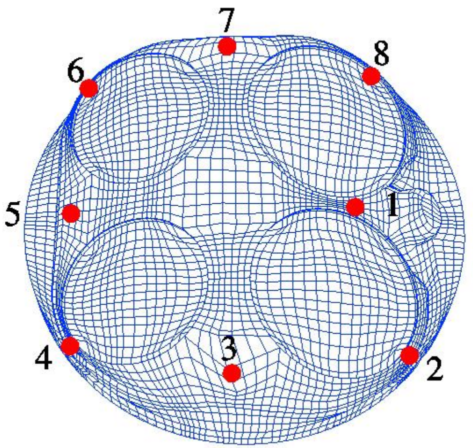
Liang, 2007

Knocking combustion in SI engines

Simulated local pressures are filtered by a Butterworth band-pass filter
Pass-band frequencies used: 5~25 kHz

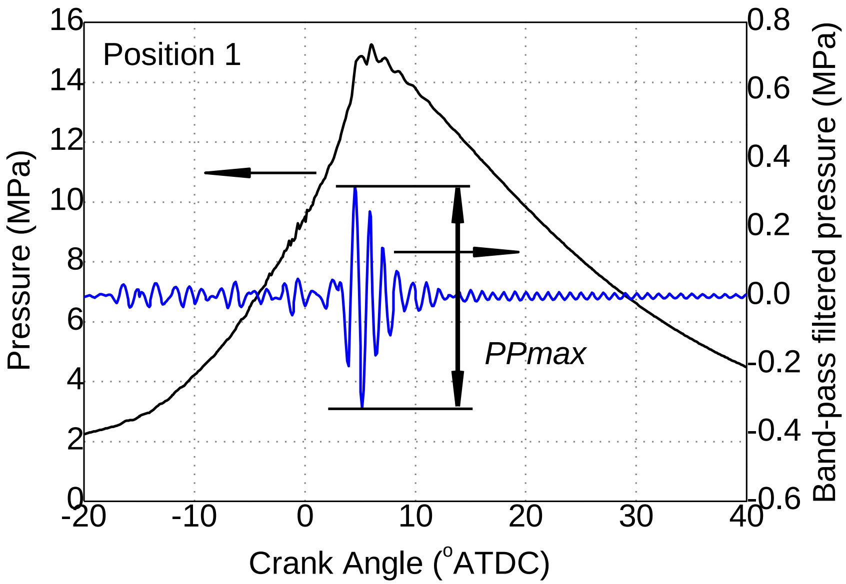
Resonant frequencies based on classical wave equation (C. Draper 1938) :

$$f_{m,n} = \alpha_{m,n} \frac{c_s}{\pi B}$$



Numerical Transducers

Resonant frequency	f_{10}	f_{20}	f_{01}	f_{30}	f_{40}	f_{11}
Analytical value (kHz)	6.7	11.2	14.0	15.4	19.4	19.5



Knock Index: $$KI = \frac{1}{N}\sum_{n=1}^{N} PP_{\max,n}$$

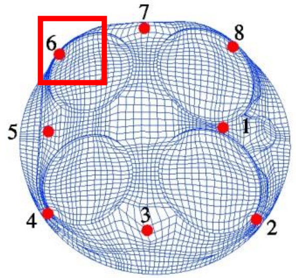
Power Index: $$PI = \frac{1}{V_{disp}}\int_{V_1}^{V_2} p\,dV$$

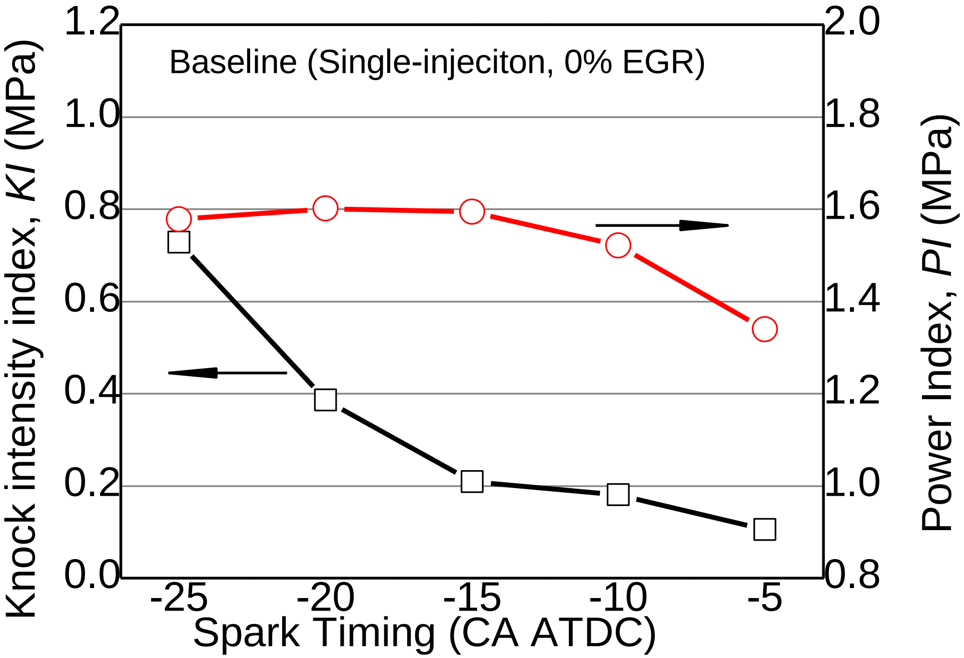
Liang, 2007

Knocking combustion in SI engines

Baseline conditions

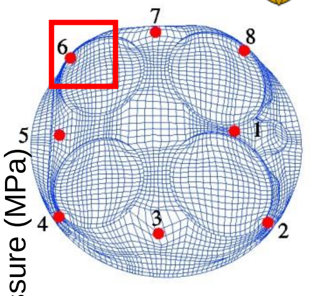
Operating mode	Direct Injection
Engine Speed	1500 rev/min
Boost pressure	160 kPa
EGR	0%
Equivalence ratio	Stoichiometric
Injection timing	-270 ATDC
Spark timing	-25,-20,-15,-10 ATDC

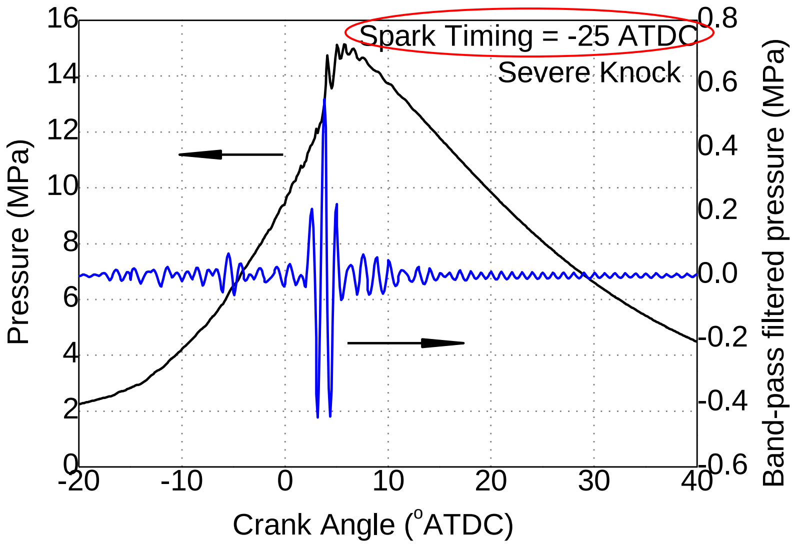


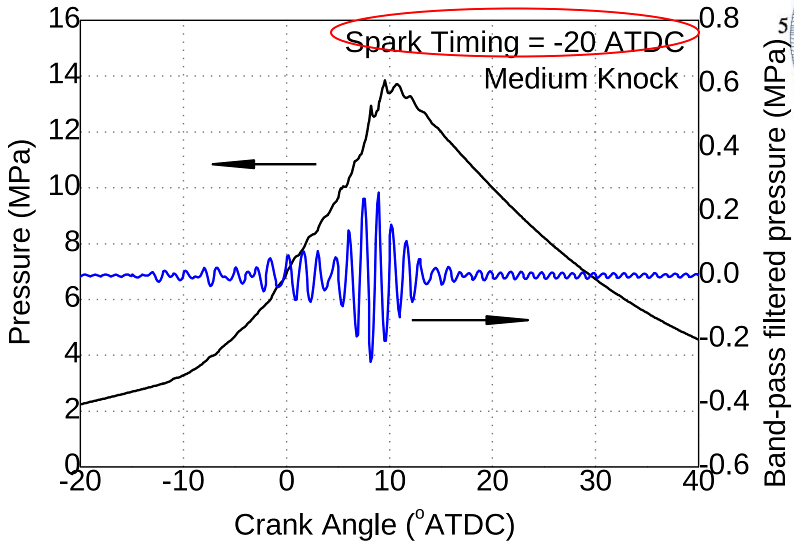


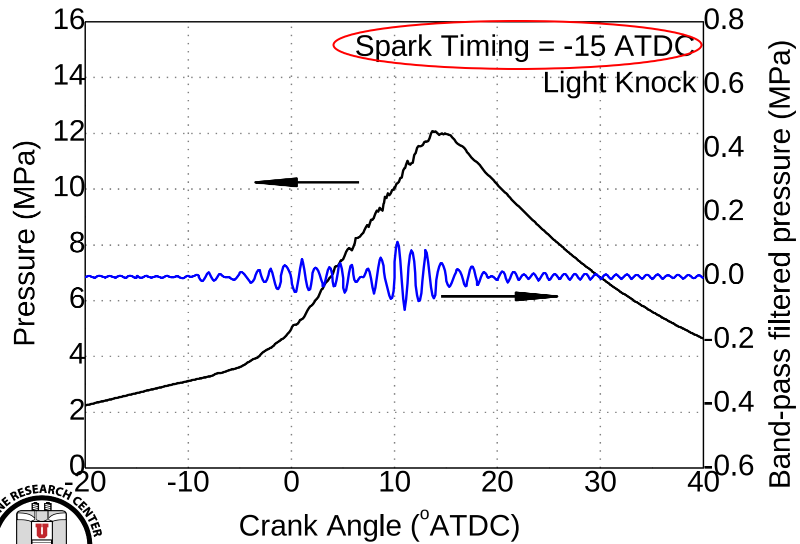
Liang, 2007

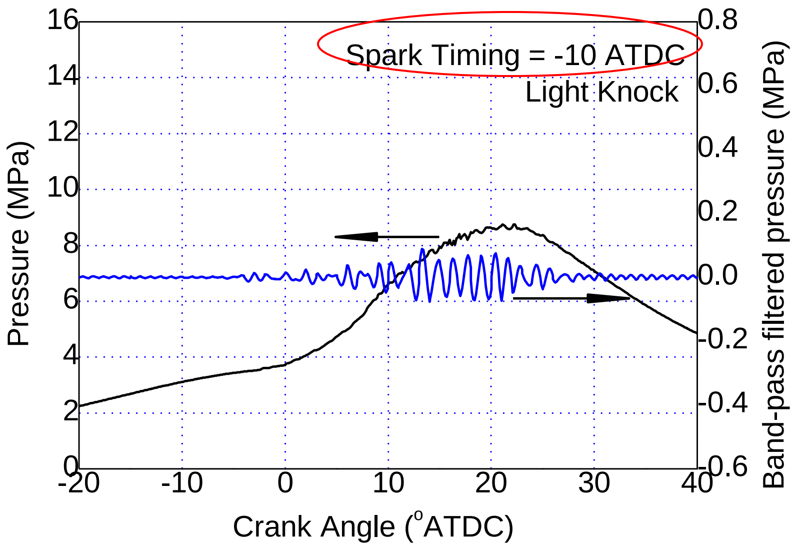
Knocking combustion in SI engines





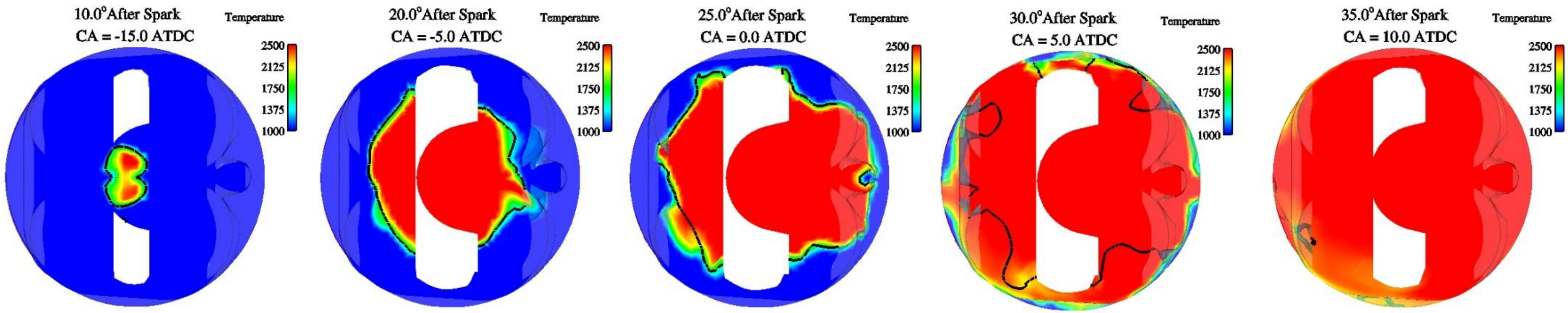




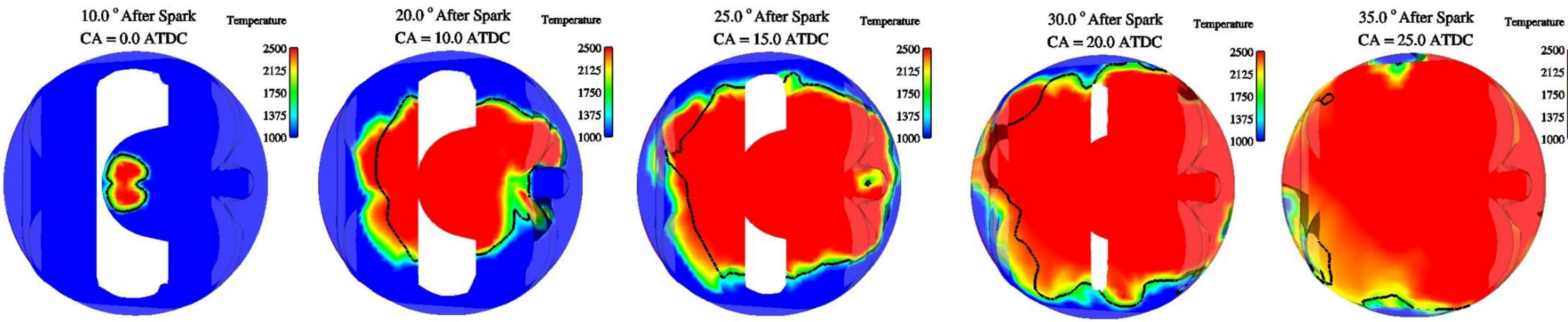


Liang, 2007

Knocking combustion in SI engines



Spark timing=-25 ATDC Severe knock

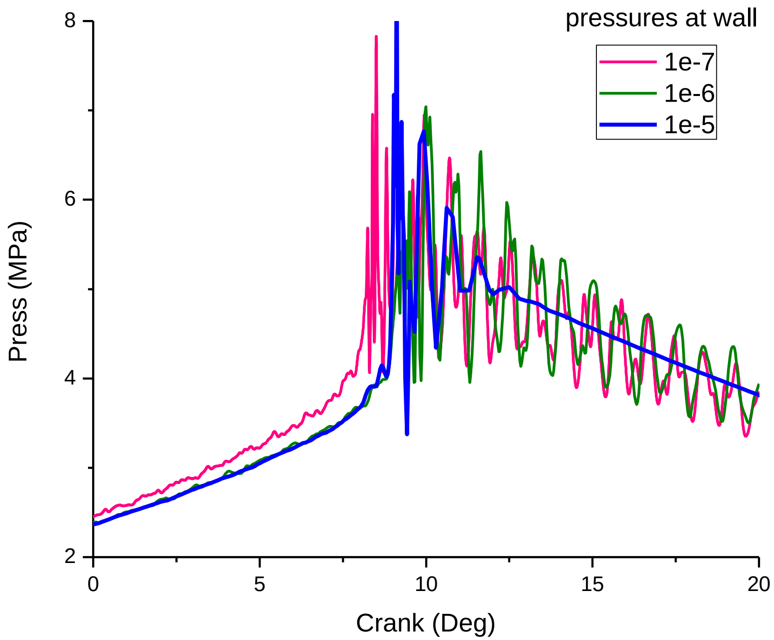


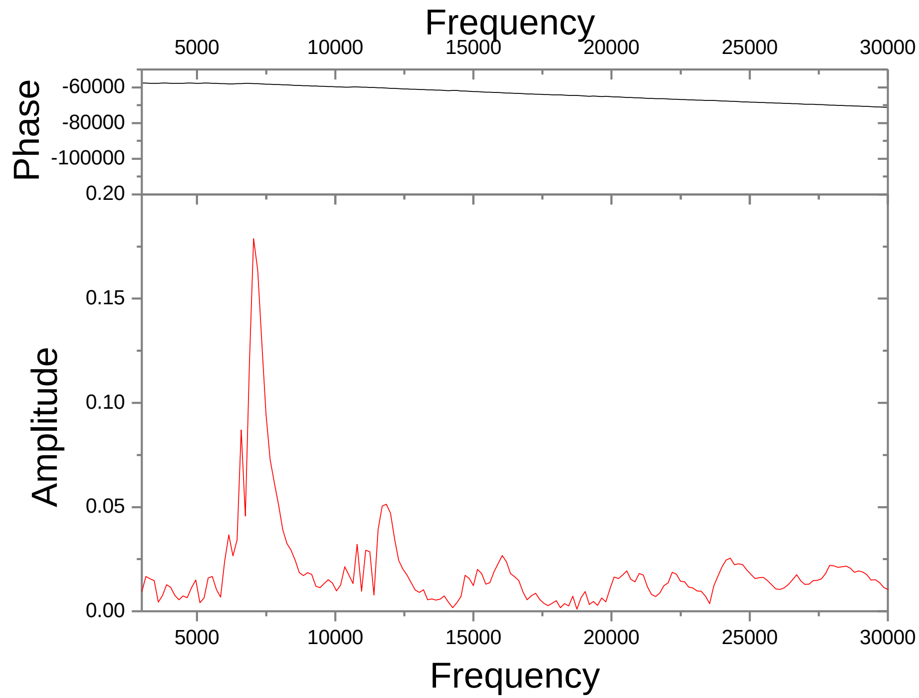
Spark timing=-10 ATDC Light knock

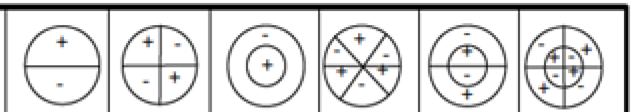
Factors affecting knock intensity:
End-gas auto-ignition tendency; Piston movement.

Wang, 2013

Pressure oscillations during knock





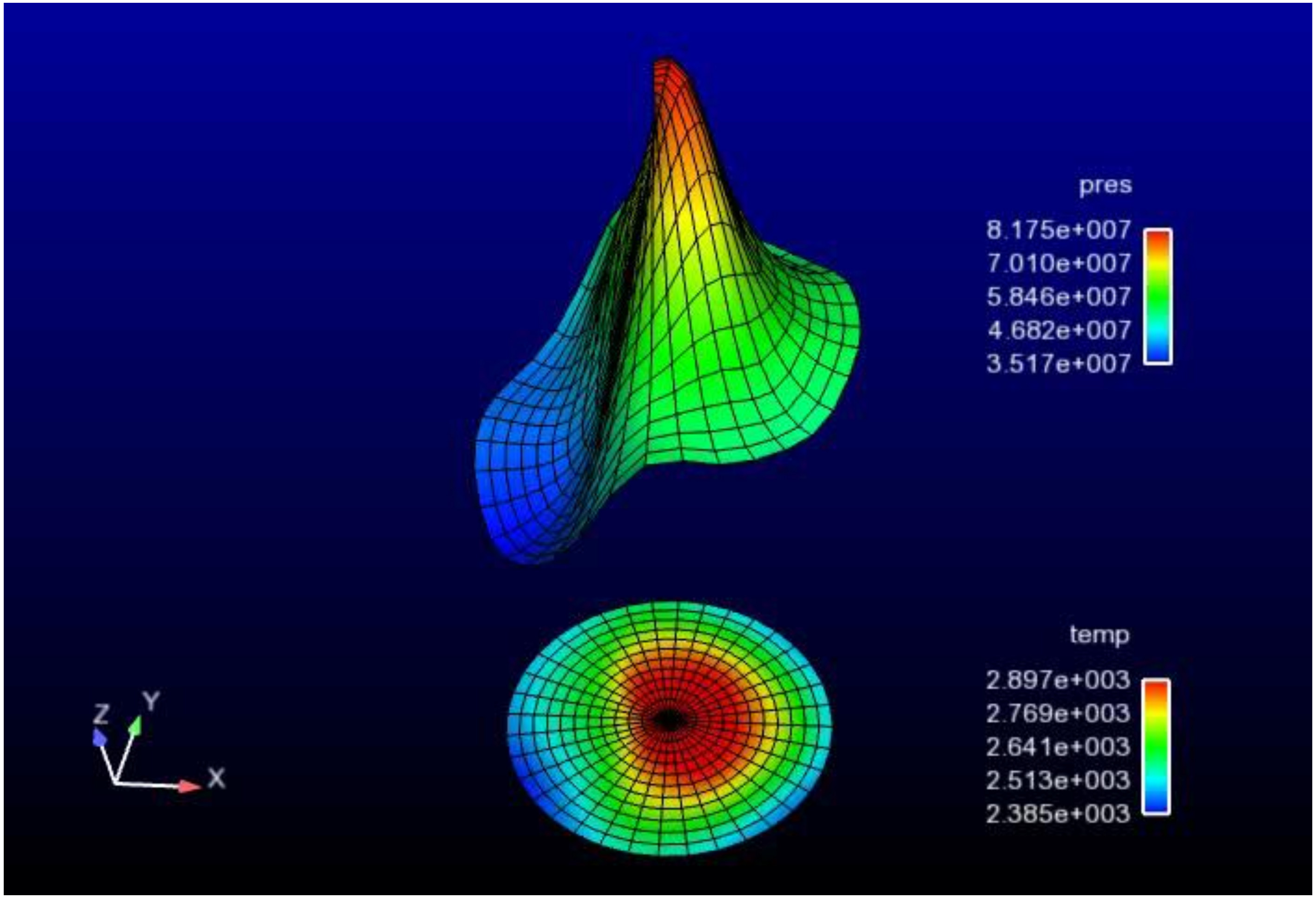


(m,n)	1,0	2,0	0,1	3.0	1,1	2,1
$\rho_{m,n}$	1.84	3.05	3.83	4.20	5.33	6.71
$f_{m,n}(kHz)$	5.01	8.31	10.43	11.43	14.51	18.25
	6.8	11.4	14.3	15.6	19.8	25.0

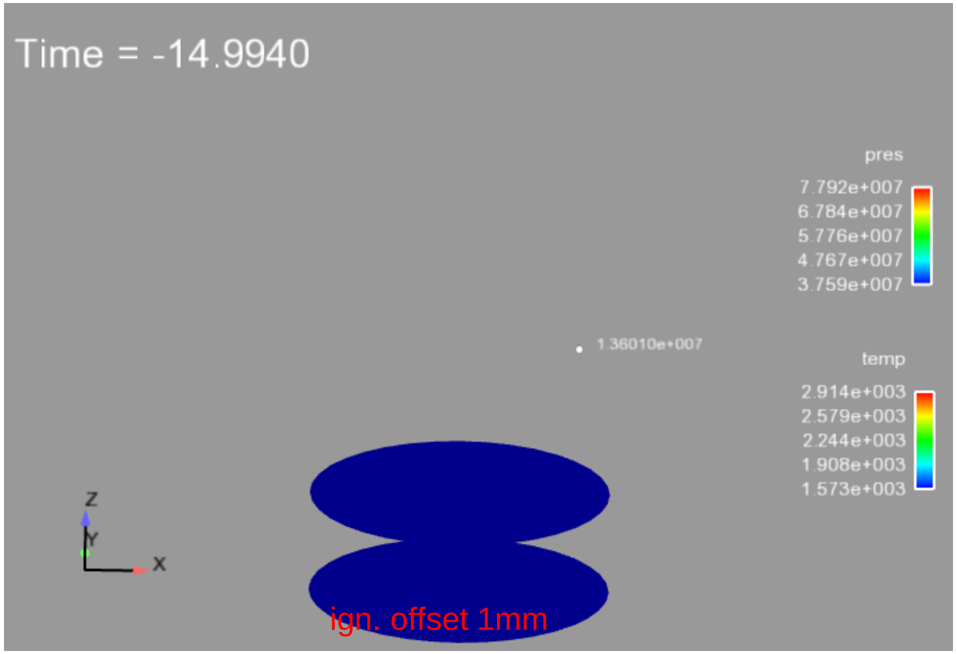
Power spectrum shows high energy in 3rd circumferential mode

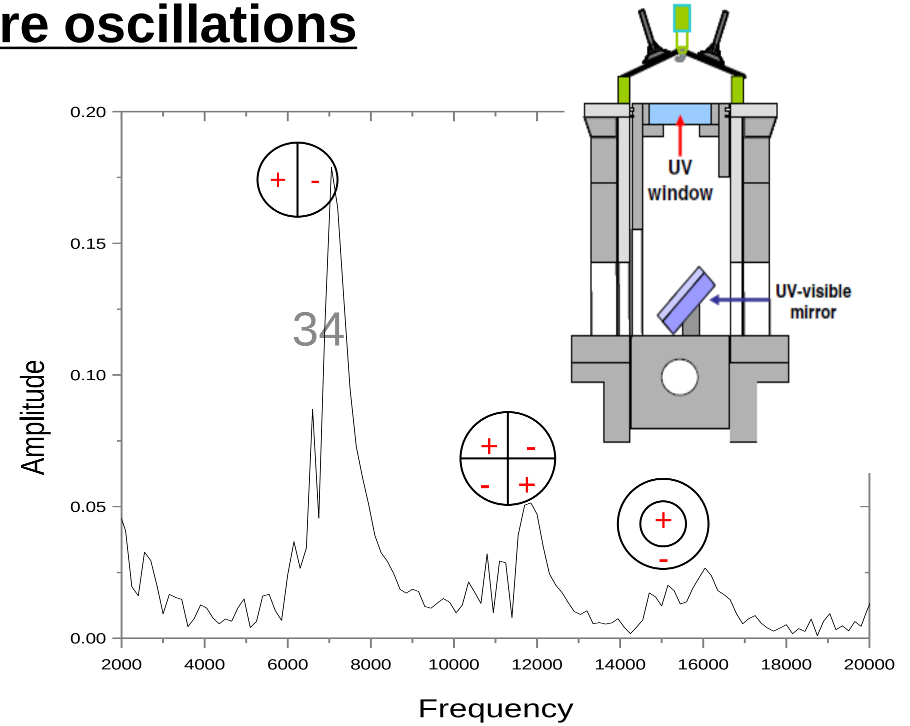
Wang, 2013

Pressure oscillations during knock



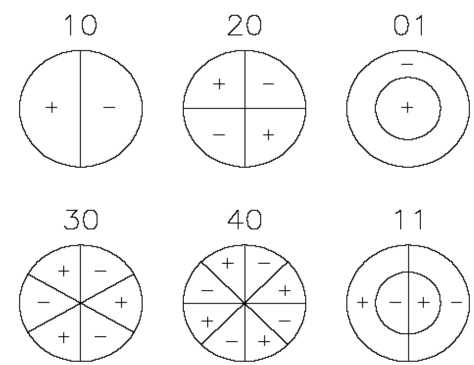
Acoustic characteristics of pressure oscillations





Knocking oscillation is mainly from 1st resonant mode - oscillating energy is focused at 7.2 kHz.

Although resonances also occur at 12.0, 15.0 and 16.4 kHz, their amplitudes are much smaller than 1st resonant mode.

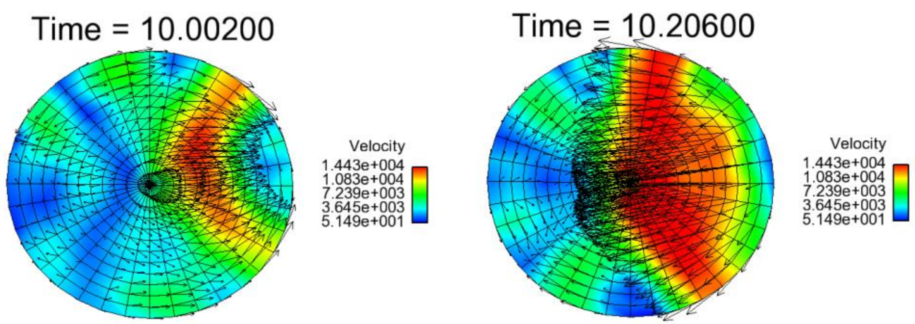


First 6 resonant frequencies

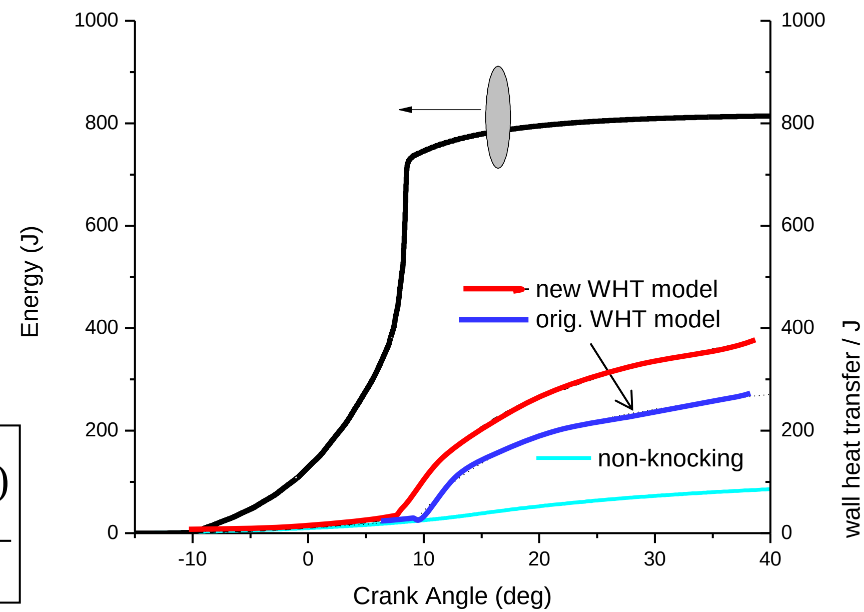
Resonant mode	f_{10}	f_{20}	f_{01}	f_{30}	f_{40}	f_{11}
Analytical Value (kHz)	7.2	12.0	15.0	16.4	20.8	26.3

Heat transfer during knock

Oscillating flow during knocking at
10.0 CA and 10.2 CA



$$q_w = \frac{\rho c_p u^* T \ln(T/T_w) + (2.1y^+ + 33.4)\dfrac{\nu}{u^*}\left(-\dfrac{1}{\gamma - 1}\dfrac{dp}{dt} + Q_c\right)}{2.1\ln(y^+) + 2.5}$$



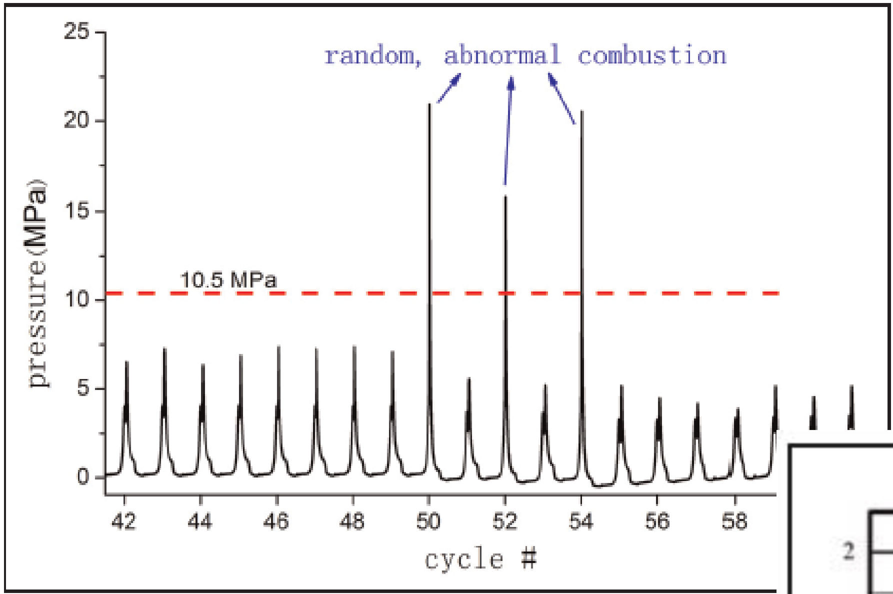
Compared to non-knocking case, engine knock significantly enhances heat transfer to walls.

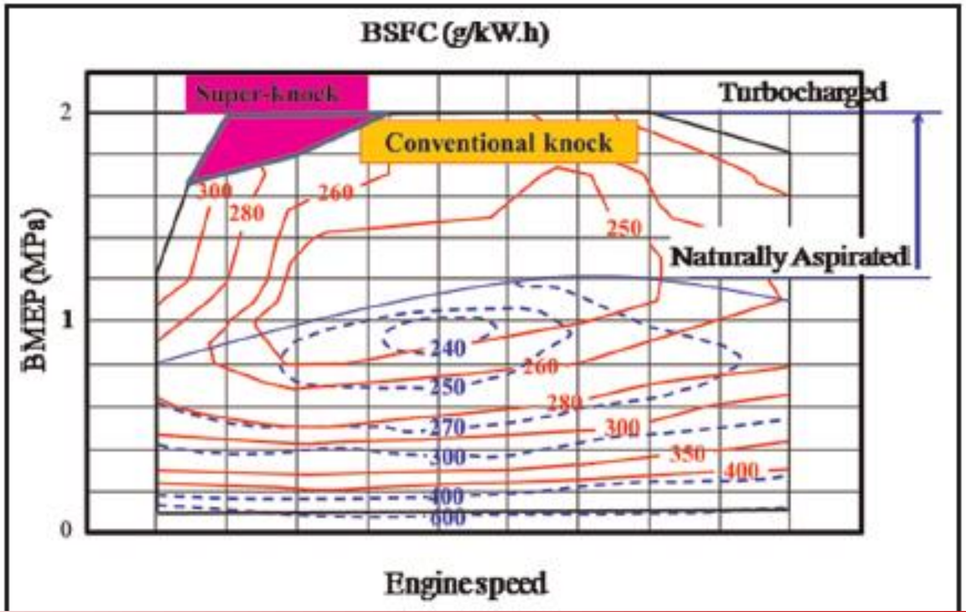
Energy loss via heat transfer during combustion period is nearly 40% of total fuel energy under heavy knocking conditions, and is nearly 4 times heat transfer of non-knocking condition.

Wang, 2014

"Superknock"

Super-knock is severe engine knock triggered by pre-ignition randomly, sometimes after many thousands of engine cycles





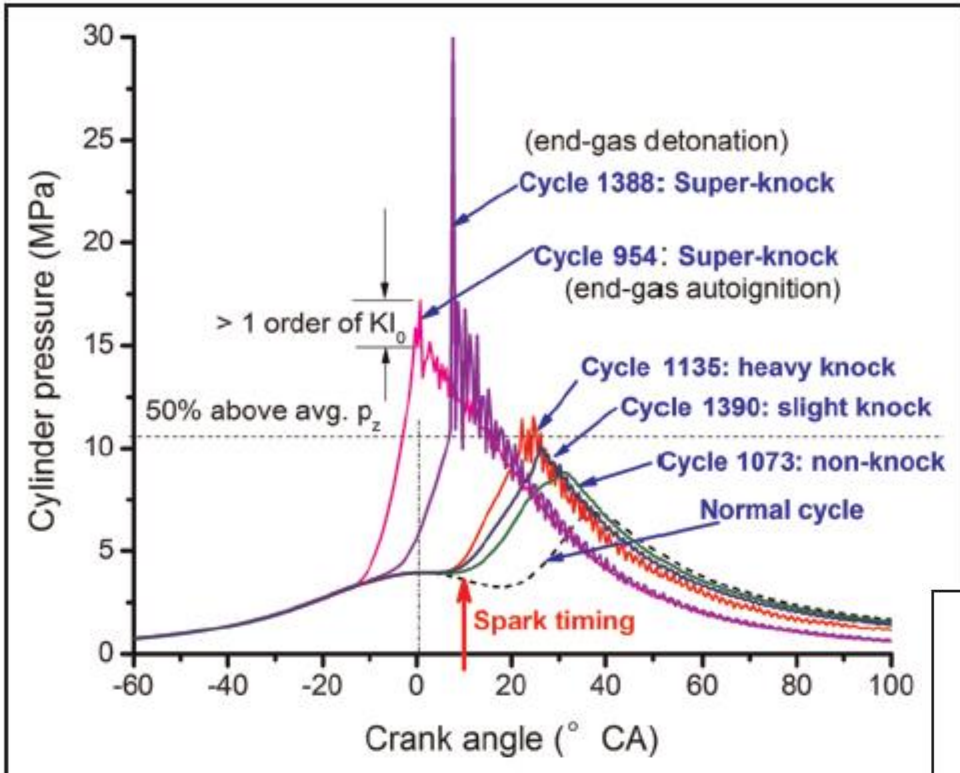
"Superknock"

Can lead to catastrophic engine damage:
(a) spark electrode breakup,
(b) exhaust valve melt, and
(c) piston ring land broken

(a) (b) (c)

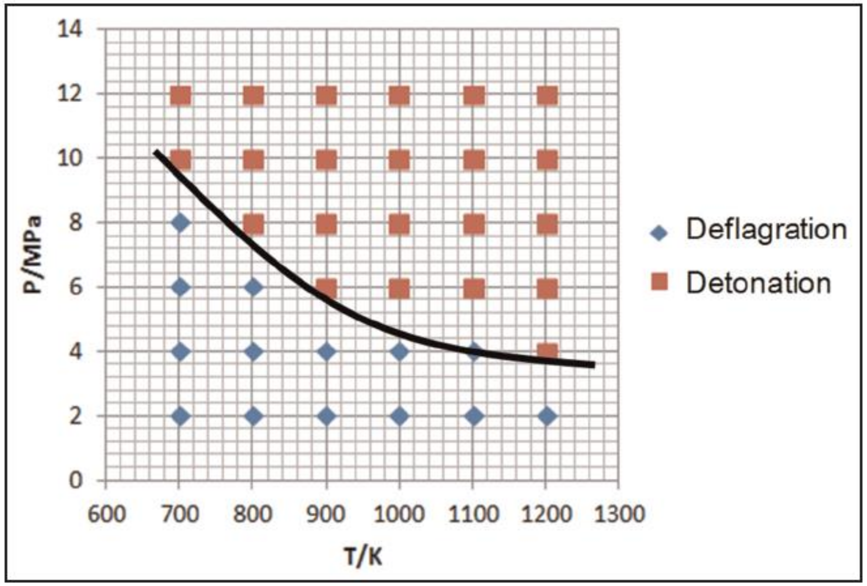
Wang, 2014

"Superknock"



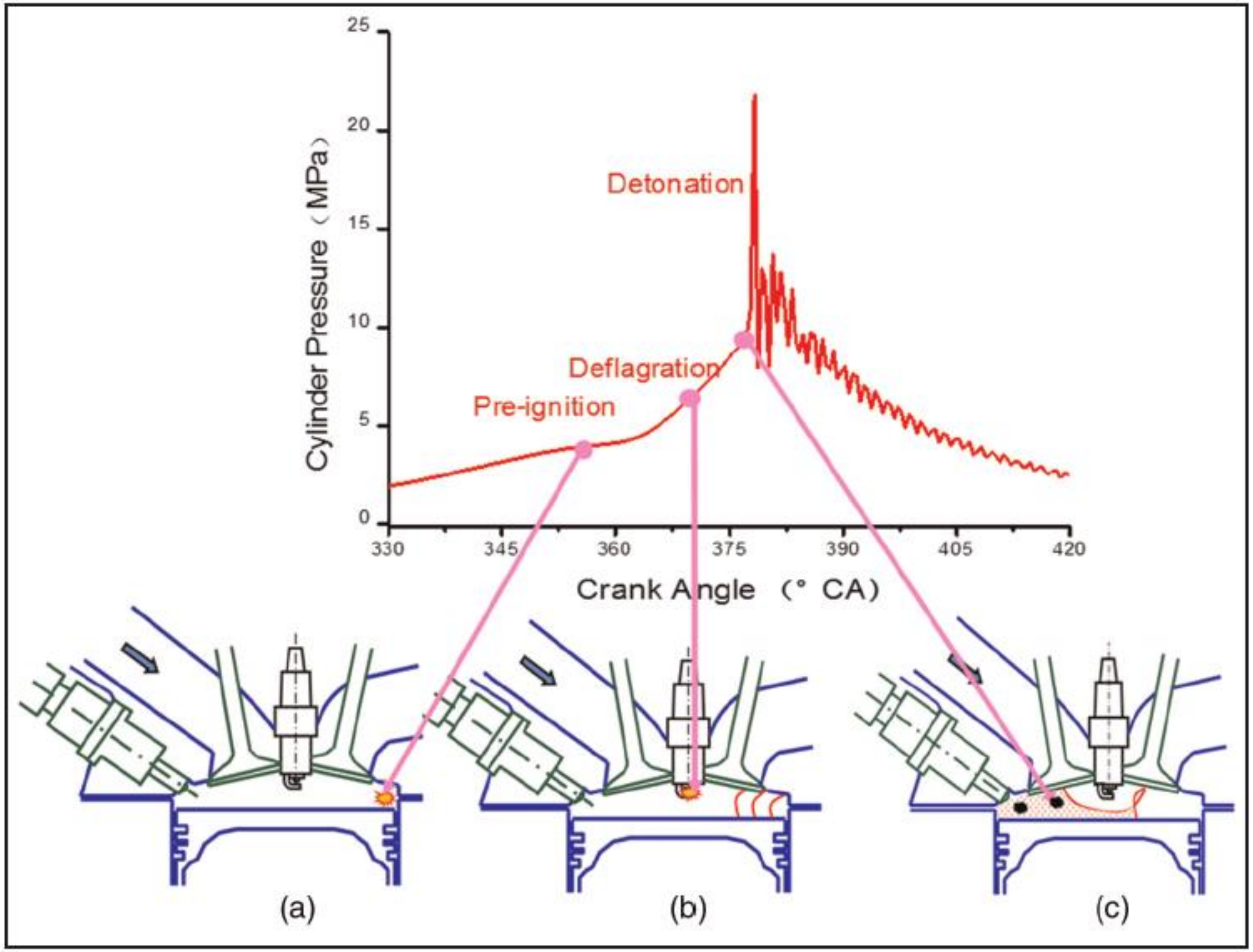
Thought to be due to pre-ignition of hot-spots from "particles/deposits"

Simulations of Deflagration-to-Detonation Transitions (DDT)



Wang, 2014

"Superknock" exacerbated in highly boosted SI engines



Ring pack design has been shown to play an important role in reducing frequency of "Superknock" events

Possible process of pre-ignition to super-knock: (a) hot-spot auto-ignition, (b) flame and spark ignition, and (c) hot-spot induced end-gas detonation.

Tan, 2004
Reitz, 2009

Summary

CFD modeling is capable of describing both diesel and spark-ignition combustion characteristics over a wide range of conditions.

Diesel (mixing-controlled) and premixed combustion is adequately represented without requiring sub-grid-scale turbulence-chemistry interactions to be modeled. The effect of turbulence on combustion is modeled satisfactorily using an integrated G-equation-based combustion model with detailed chemical kinetics (CHEMKIN).

Very similar results are achieved with and without consideration of flame propagation for diesel combustion:

- G-equation flame propagation model does reveal edge flame at lift-off location (not observed with the kinetics-only calculation)

Flame-propagation-dominated premixed charge spark-ignition engine combustion requires specification of turbulent flame speed in the model.

The G-equation-CHEMKIN model allows all combustion regimes to be modeled (**GAMUT**: G-equation for All Mixtures – a Universal Turbulent combustion model – Tan & Reitz, 2004, Reitz & Sun, 2009).

Integration with chemistry model allows model to predict both diesel ignition and SI engine knock processes.