Reciprocating Internal Combustion Engines

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

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

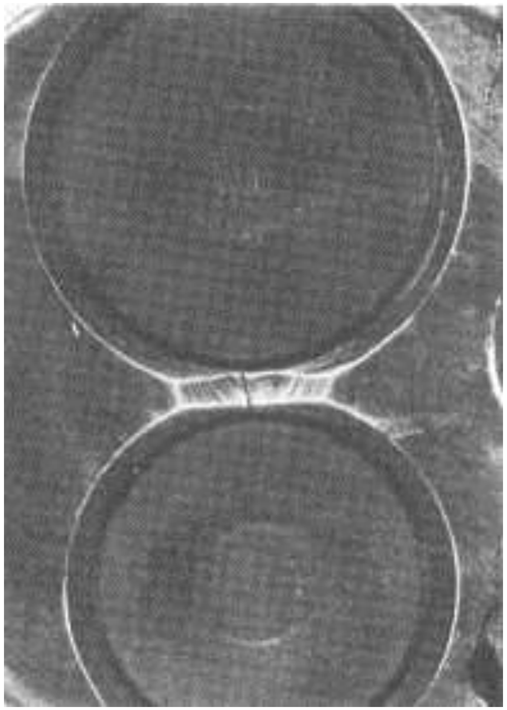
Challen, 1998

Engine heat transfer

Up to 30% of the fuel energy is lost to wall heat transfer
Can influence engine ignition/knock
Engine durability – catastrophic engine failure

Scorching

Detonation



Cracking

Part 4: Heat transfer, NOx and Soot Emissions

Han, 1995
Wang, 2012

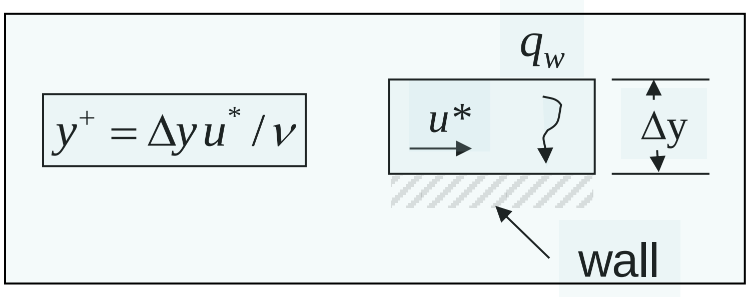
Heat transfer

Gas phase energy equation

$$\frac{\partial(\rho I)}{\partial t} + \nabla\cdot(\rho \mathbf{u} I) = -p\nabla\cdot\mathbf{u} - \nabla\cdot\mathbf{J} + \rho\varepsilon + \dot{Q}^c + \dot{Q}^s + \dot{Q}^r$$

Radiation source term

$$\dot{Q}^r(\mathbf{r}) = \kappa\left[\int_{\mathbf{\Omega}=4\pi} I(\mathbf{r},\mathbf{\Omega})\,d\mathbf{\Omega} - 4\pi I_b(\mathbf{r})\right]$$



Wall heat flux (account for compressibility)

With radiation	Without radiation
$q_w = \dfrac{\rho_g C_p u^* T_g \ln(T_g/T_w) - (2.1y^+ + 33.34) G \upsilon/u^*}{2.1\ln(y^+) + 2.5}$	$q_w = \dfrac{\rho C_p u^* T_g \ln(T_g/T_w)}{2.1\ln(y^+) + 2.5}$
$\dfrac{dT}{dy} = \dfrac{q_w}{\rho_g C_p \nu}\left(\dfrac{2.1}{y^+} + 2.1G^+\right)$	$\dfrac{dT}{dy} = \dfrac{2.1u^* T_g \ln\left(T_g/T_w\right)}{\upsilon y^+\left[2.1\ln(y^+) + 2.5\right]}$

G radiative heat flux = q_w^r

Wiedenhoefer, 2003

Radiation modeling

Radiation Transfer Equation:

$$(\mathbf{\Omega}\cdot\nabla)I(\mathbf{r},\mathbf{\Omega}) = -(a_{net}+\sigma_s)I(\mathbf{r},\mathbf{\Omega}) + \kappa I_b(\mathbf{r}) + \frac{\sigma_s}{4\pi}S(\mathbf{r},\mathbf{\Omega})$$

a_{net} net absorption coefficient, σ_s scattering coefficient

$\kappa = a_{net} + \sigma_s$ extinction coefficient

Back body radiative flux (independent of angle) $I_b(\mathbf{r}) = \dfrac{\sigma T_w^4}{\pi}$

Scattering terms, σ_s, S ~ usually neglected compared to absorption

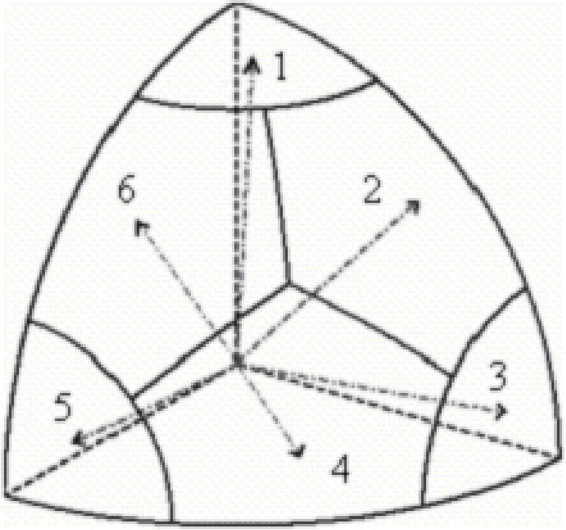
Radiation intensity at wall

$$G = q_w^r = \varepsilon \int_{\mathbf{n}\bullet\mathbf{\Omega}'<0} |\mathbf{n}\bullet\mathbf{\Omega}'| I(\mathbf{r},\mathbf{\Omega}')\,d\mathbf{\Omega}' - \varepsilon\sigma T_w^4$$

ε surface emissivity

Discrete ordinates model

$$\dot{Q}^r(\mathbf{r}) = \kappa\left[\sum_{m=1}^{nDir}\varpi^m I^m(\mathbf{r}) - 4\pi I_b(\mathbf{r})\right]$$



(e) Spherical surface division for S_6

Wiedenhoefer, 2003a

Soot and gas absorption

Total absorption coefficient

$$a_{net} = a_{soot} + a_{CO_2+H_2O}$$

$$a_g\left(T,P,L_e\right) = \frac{1}{L_e}\ln\left[1-\varepsilon_g\left(T,P,L_e\right)\right]$$

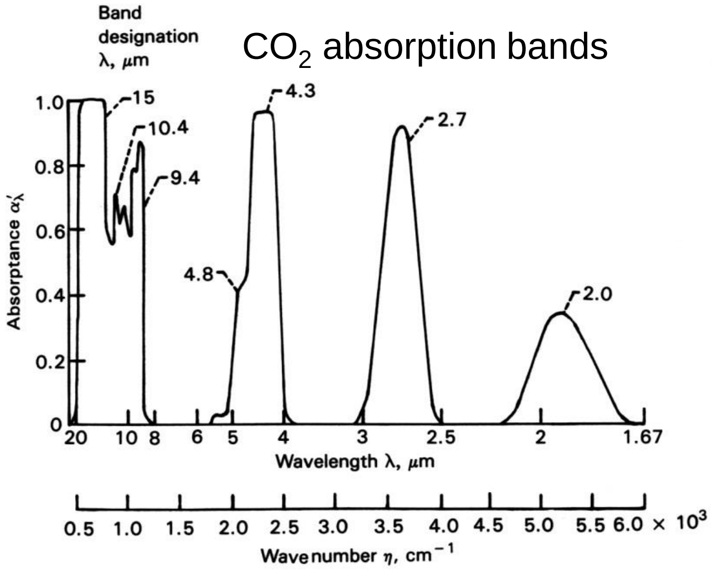
$$\varepsilon = 1-\left(1-\varepsilon_{fuel}\right)\left(1-\varepsilon_{CO}\right)\left(1-\varepsilon_{CO_2}\right)\left(1-\varepsilon_{H_2O}\right)$$

Soot absorption

$$a_{soot} = 1260 C_{soot} T \text{ m}^{-1}$$

Wide band model for CO_2 and H_2O

$$\varepsilon_{b\eta}\left(\eta_{band\ center}, T\right) = \left(\frac{2C_1\eta^3}{e^{C_2\eta/T}-1}\right)_{band\ center}$$


CO_2 absorption bands

Importance of soot:

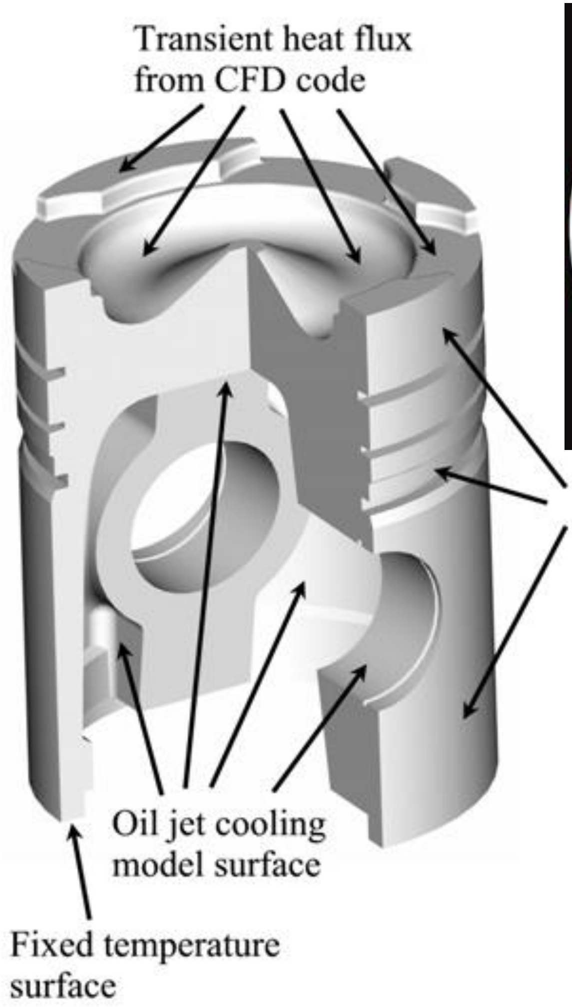
$$a_{gas} \propto \frac{1}{T} \qquad a_{soot} \propto T$$

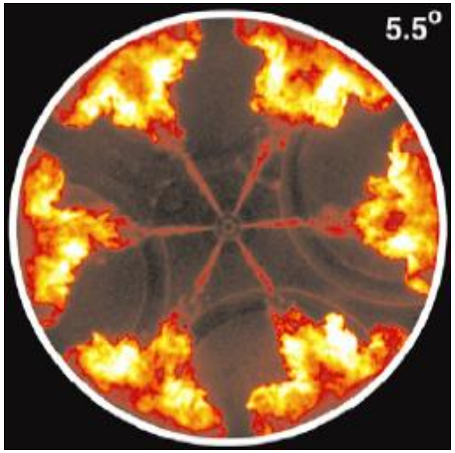
$$\dot{Q}^r(\mathbf{r}) = a\left[\int_{\Omega=4\pi} I(\mathbf{r},\mathbf{\Omega})\,d\mathbf{\Omega} - 4\pi I_b(\mathbf{r})\right] \propto \left[a_{gas}+a_{soot}\right]\sigma T^4 \propto \sigma\left[T_{gas}^3 + T_{soot}^5\right]$$

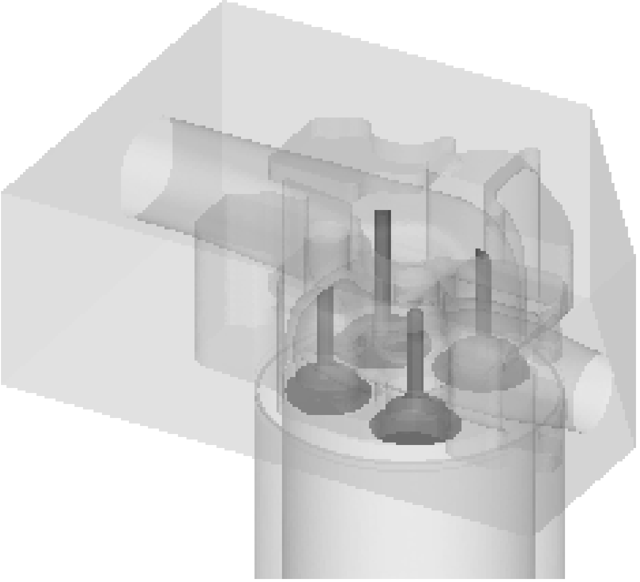
Wiedenhoefer, 2000

Wall heat transfer

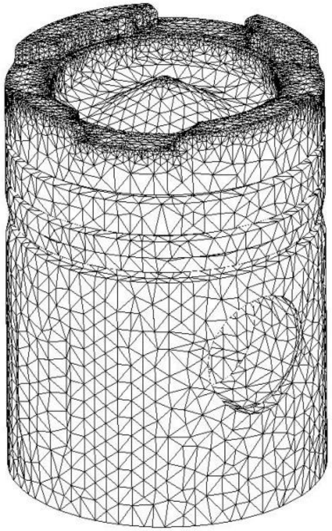
Conjugate heat transfer modeling
ERC - Heat Conduction in Components code (HCC)







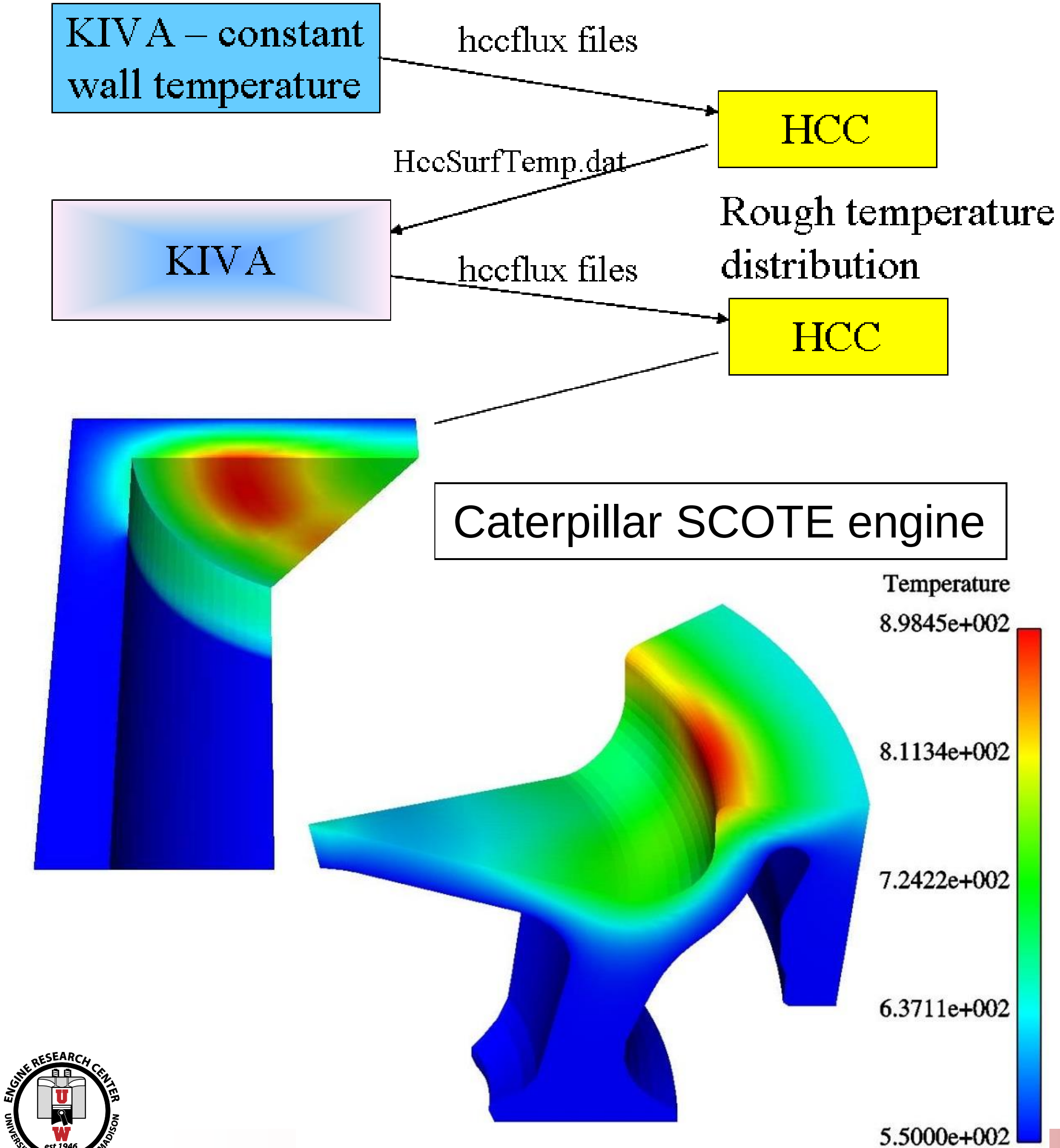
Iterative coupling between HCC and CFD code



Unstructured HCC Mesh

Wiedenhoefer, 2000

Wall heat transfer


KIVA – constant wall temperature

hccflux files

HCC

HccSurfTemp.dat

KIVA

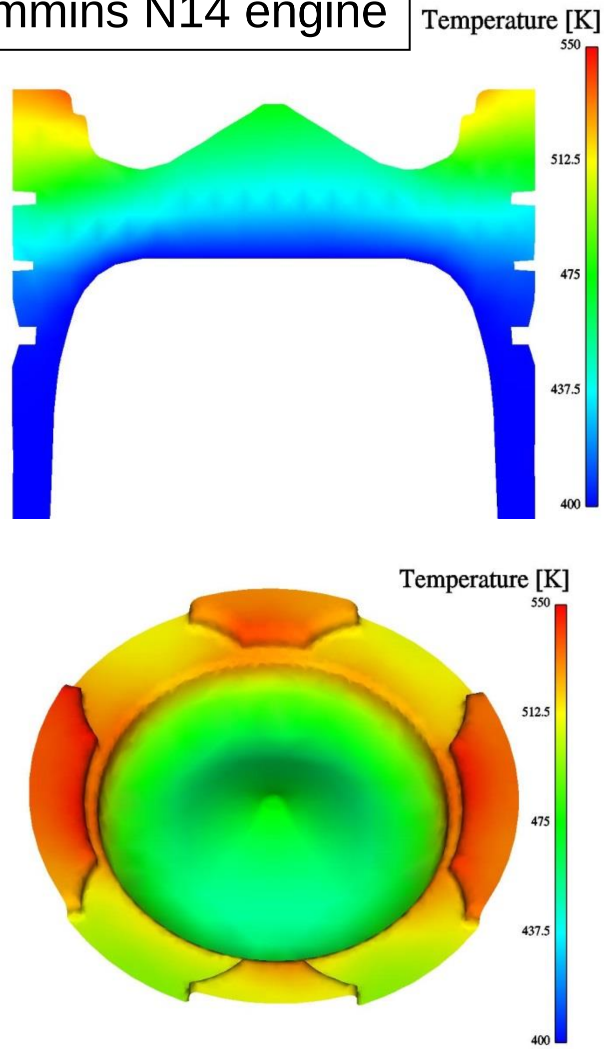
hccflux files

Rough temperature distribution

HCC

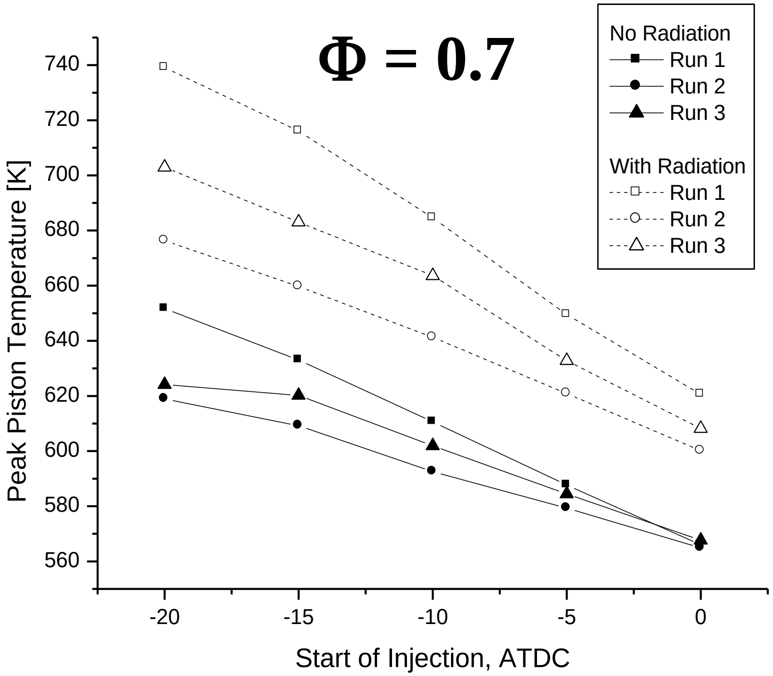
Caterpillar SCOTE engine

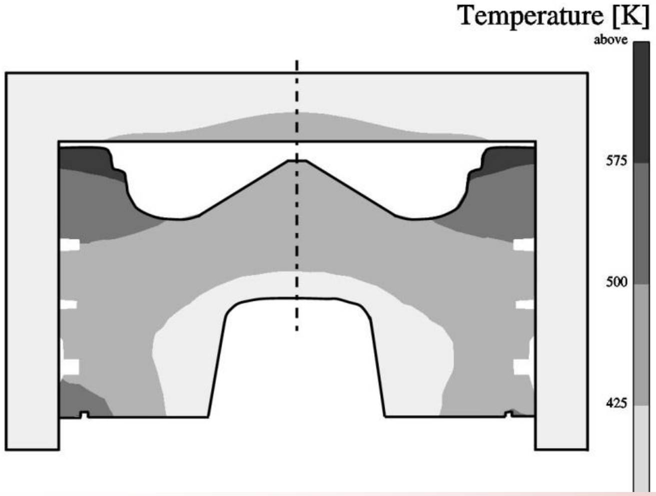
Cummins N14 engine



Wiedenhoefer, 2003

Predicted piston temperature - CDC





Effect of radiation on wall heat loss

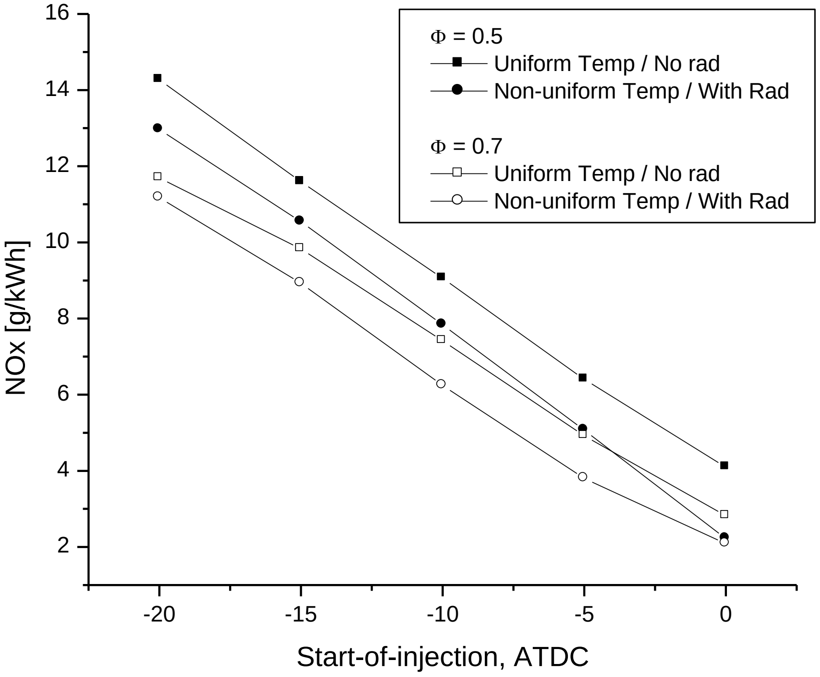
Total heat loss increased by 30% due to radiation.

34% - head, 19% - liner, 47% - piston.

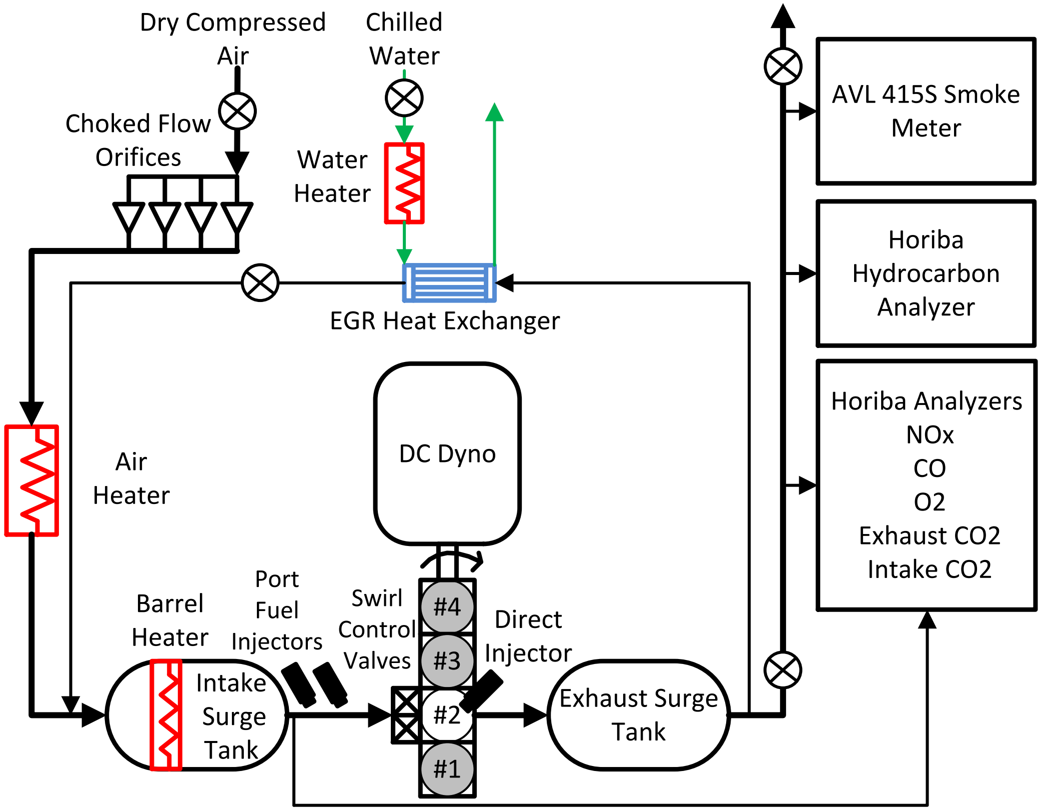
Lowers bulk gas temperatures

Results in lower NOx and higher soot

NOx reduced by as much as 30% (ave)



Wall heat flux measurements

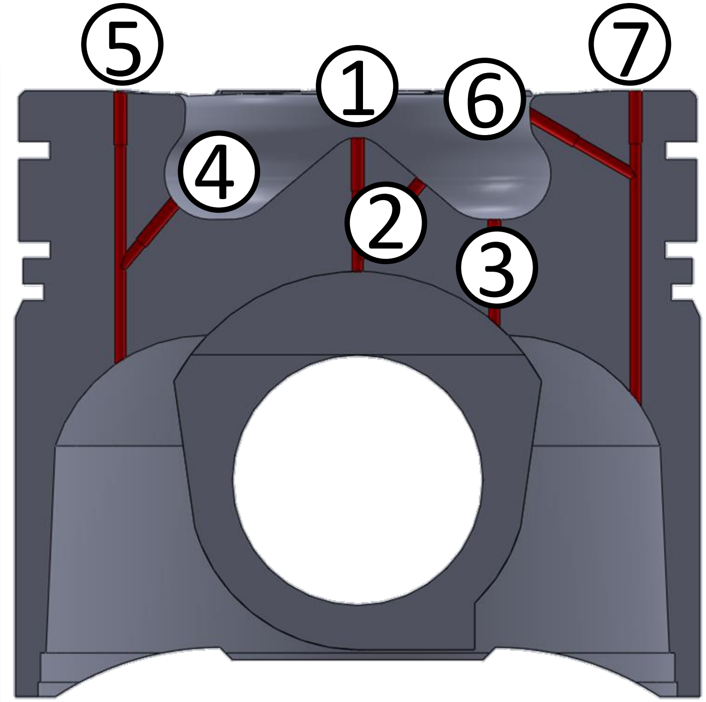


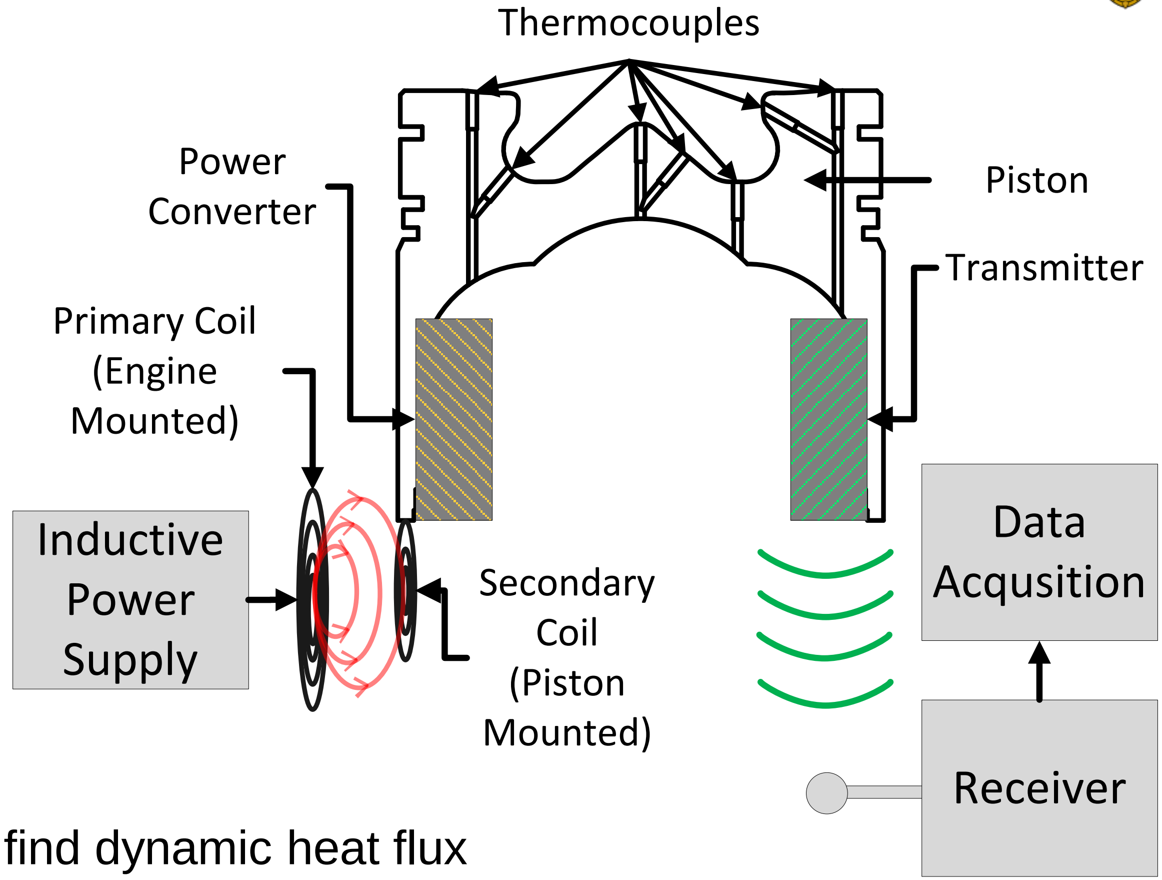
4-cylinder engine head
cylinder #1,3,4 deactivated

Engine Geometry	
Base Engine	GM 1.9L Diesel
Compression Ratio	16.3
Displacement (Liters)	0.477
Stroke (mm)	90.4
Bore (mm)	82
Intake Valve Closing	-132° aTDC
Exhaust Valve Opening	112° aTDC
Swirl Ratio	1.5 -4.8
Piston Bowl Type	Stock (Re-entrant)
Port Fuel Injectors	
Included Spray Angle	20°
Injection Pressure (bar)	2 to 10
Rated Flow (cc/sec)	< 10
Bosch Common Rail Injector	
Number of Holes	7
Hole Diameter (mm)	0.14
Included Spray Angle	155°
Injection Pressure (bar)	250 to 1000 bar

Part 4: Heat transfer, NOx and Soot Emissions

Gingrich, 2014





- Fourier analysis is applied to find dynamic heat flux
- Integral of the dynamic heat flux over the full cycle is zero

$$T(t) = T_m + \sum [A_n \cos(n\omega t) + B_n \sin(n\omega t)]$$

$$\longrightarrow \dot{q} = \overbrace{\frac{k}{l}(T_m - T_l)}^{\text{Steady}} + \overbrace{k\sum_{n=1}^{N}\sqrt{\frac{n\omega}{2\alpha}}[(A_n + B_n)\cos(n\omega t) - (A_n - B_n)\sin(n\omega t)]}^{\text{Dynamic}}$$

Combustion strategy effects - CDC / HCCI / RCCI

	Mode 1	**Mode 2**	**Mode 3**	**Mode 4**
Speed (RPM)	1490	1900	2300	2300
IMEPg (bar)	4.2	5.7	5.7	8
CA50 (degATDC)	4	5	4.5	8
Swirl	1.5	1.5	1.5	1.5
Intake Temperature (C)	75	50	50	35
Intake Pressure (kPa)	115	130	130	188
ERG (%)	0	0	0	55

Fuels:

Regime	**Fuel**
HCCI	91PON Gasoline / n-heptane
RCCI	F76 / 91PON Gasoline
CDC	F76

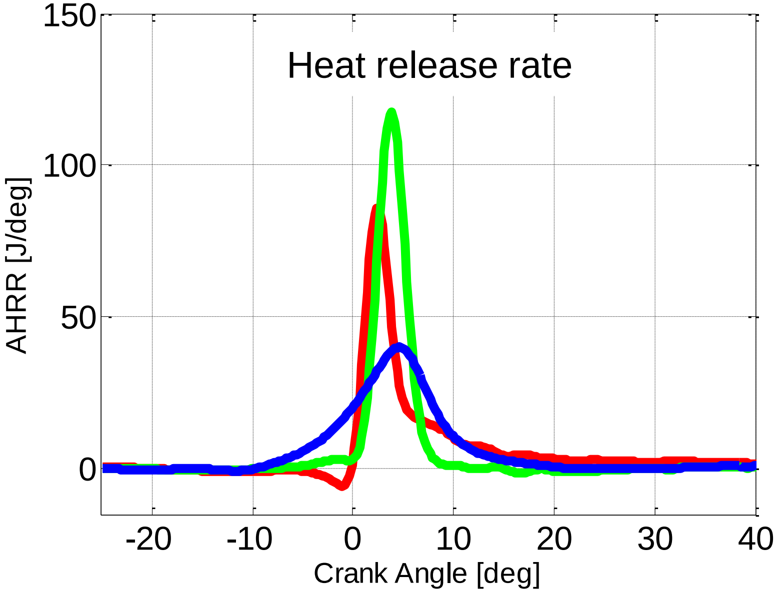
Gingrich, 2014

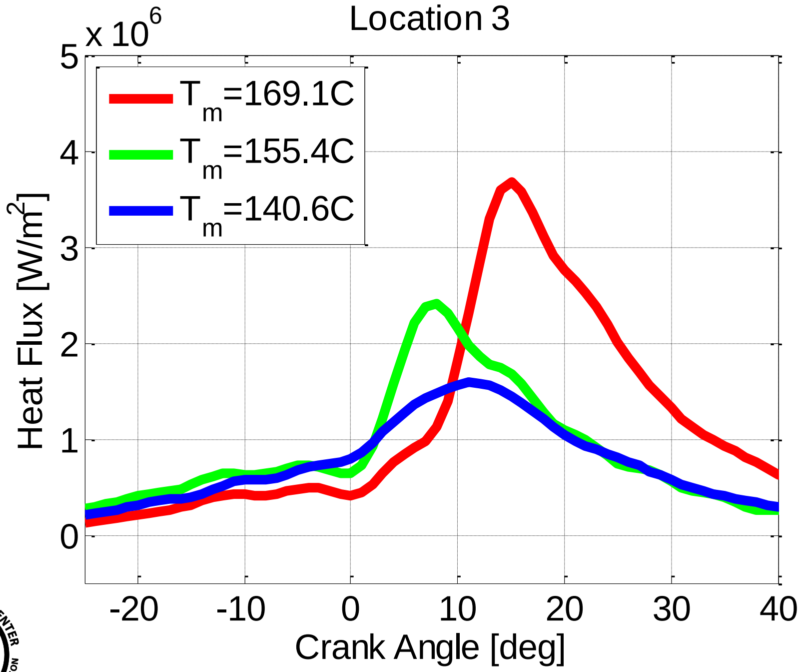
Combustion strategy effects

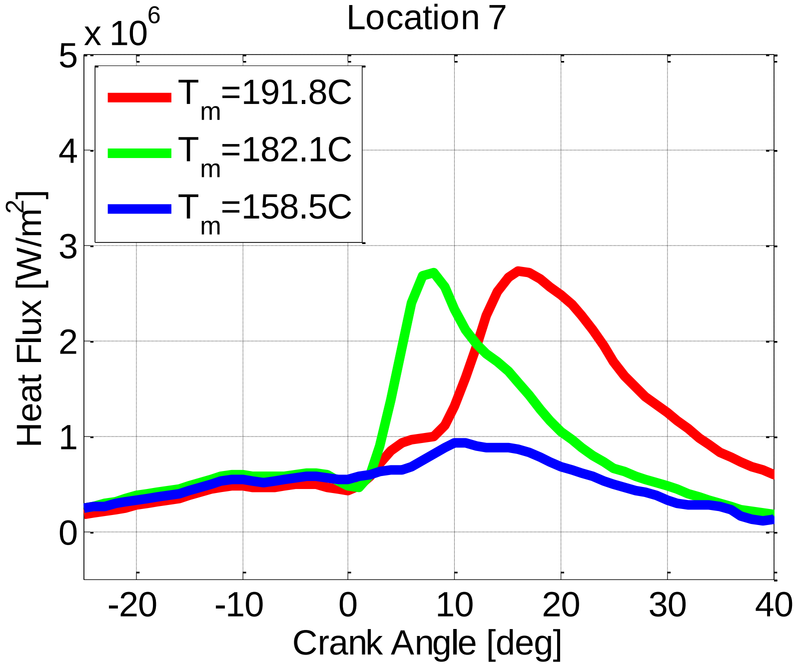
Mode 3

5.7 bar IMEPg
5 deg ATDC CA50
2300 rev/min

🟥 CDC
🟩 HCCI
🟦 RCCI

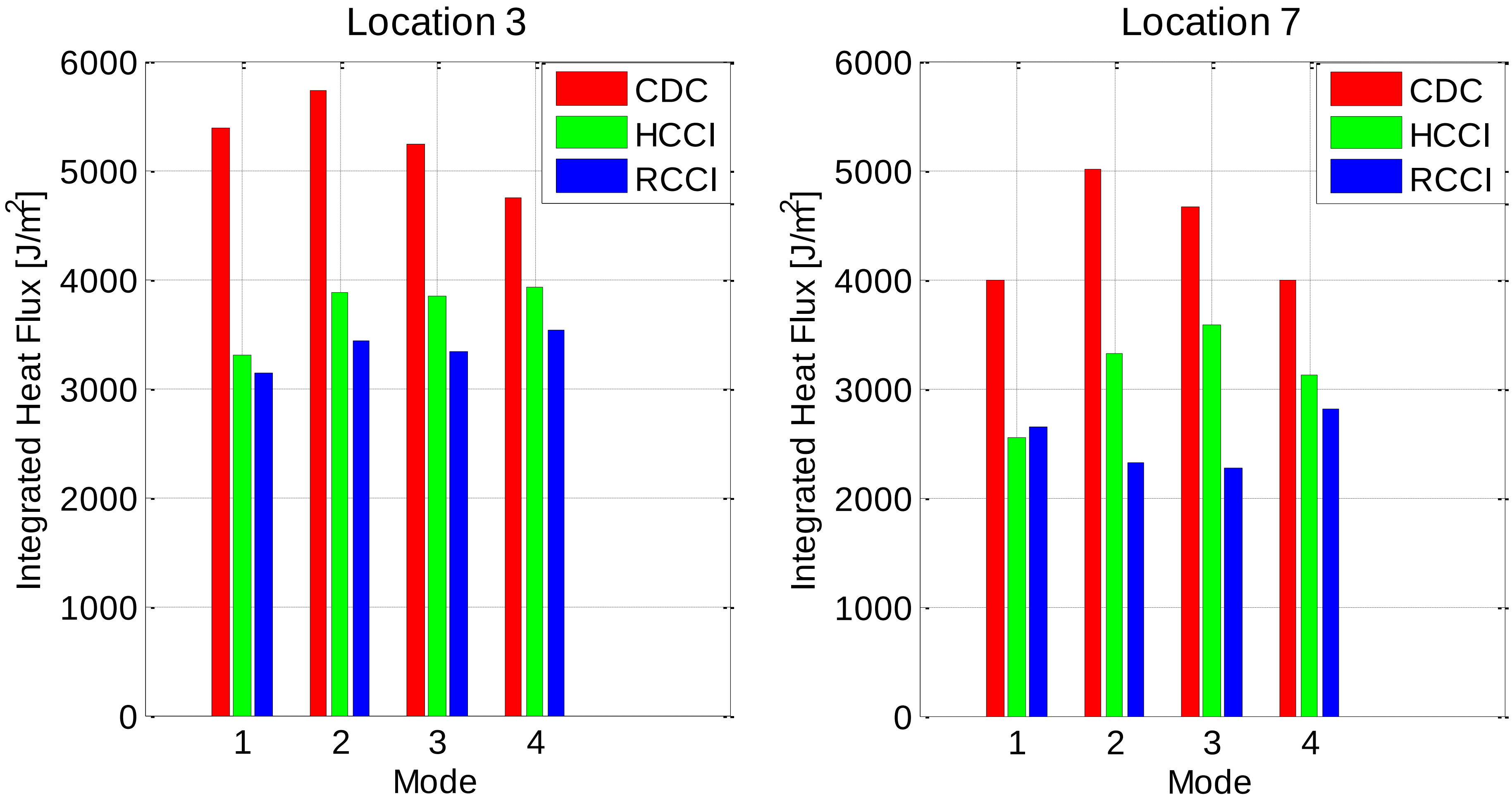






Gingrich, 2014

Combustion strategy effects - CDC / HCCI / RCCI



Heat losses significantly less with low temperature combustion strategies

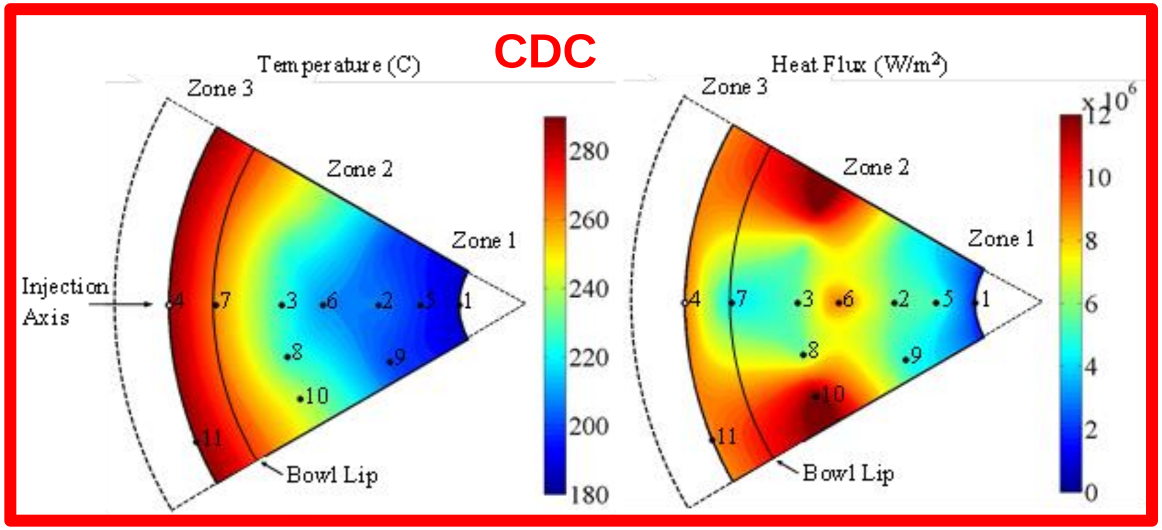
Heavy-duty diesel heat flux data

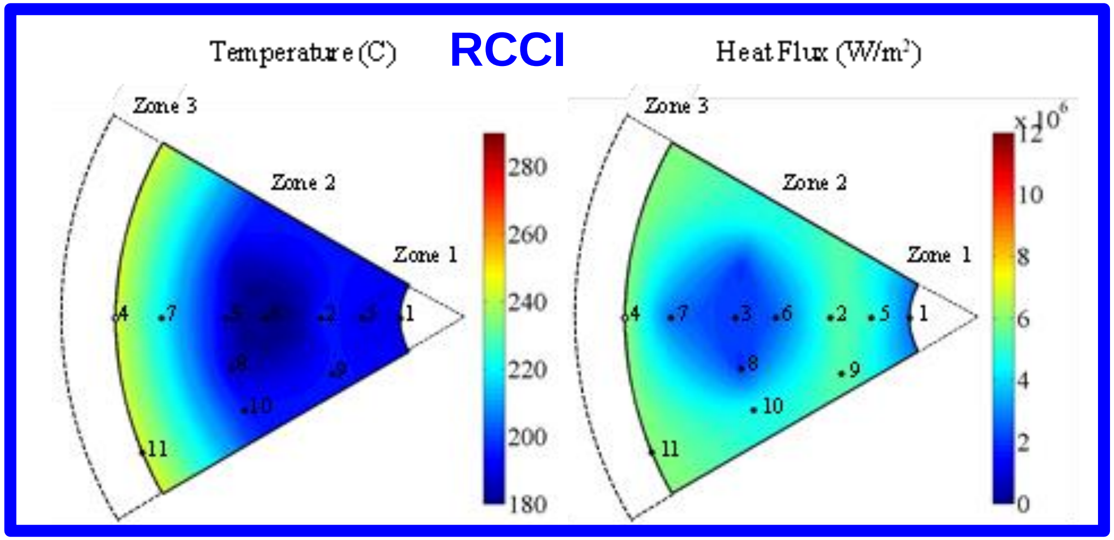
Compare CDC and RCCI combustion at matched CA50, load, Φg

(4.6°CA ATDC, 0.35)

RCCI piston heat flux measured to be lower than CDC

Area integrated HX and temp. determined





	CDC	RCCI
$\int$Piston HX fuel energy (%)	7.7	5.9
GTE (%)	51.2	52.7

Engine emissions - transportation & toxic air pollutants

Criteria air contaminants (CAC), or criteria pollutants

- air pollutants that cause smog, acid rain and other health hazards.

EPA sets standards on:

1.) Ozone ($O3$),

2.) Particulate Matter (soot):

PM10, coarse particles: 2.5 micrometers (μm) to 10 μm in size

PM2.5, fine particles: 2.5 μm in size or less

3.) Carbon monoxide (CO), 4.) Sulfur dioxide ($SO2$),

5.) Nitrogen oxides (NOx), 6.) Lead (Pb)

Toxic air pollutants - Hazardous Air Pollutants or HAPs known to cause or suspected of causing cancer or other serious health ailments.

- Clean Air Act Amendments of 1990 lists 188 HAPs from transportation.

In 2001, EPA issued Mobile Source Air Toxics Rule:

- identified 21 MSAT compounds.
- a subset of six identified having the greatest influence on health:

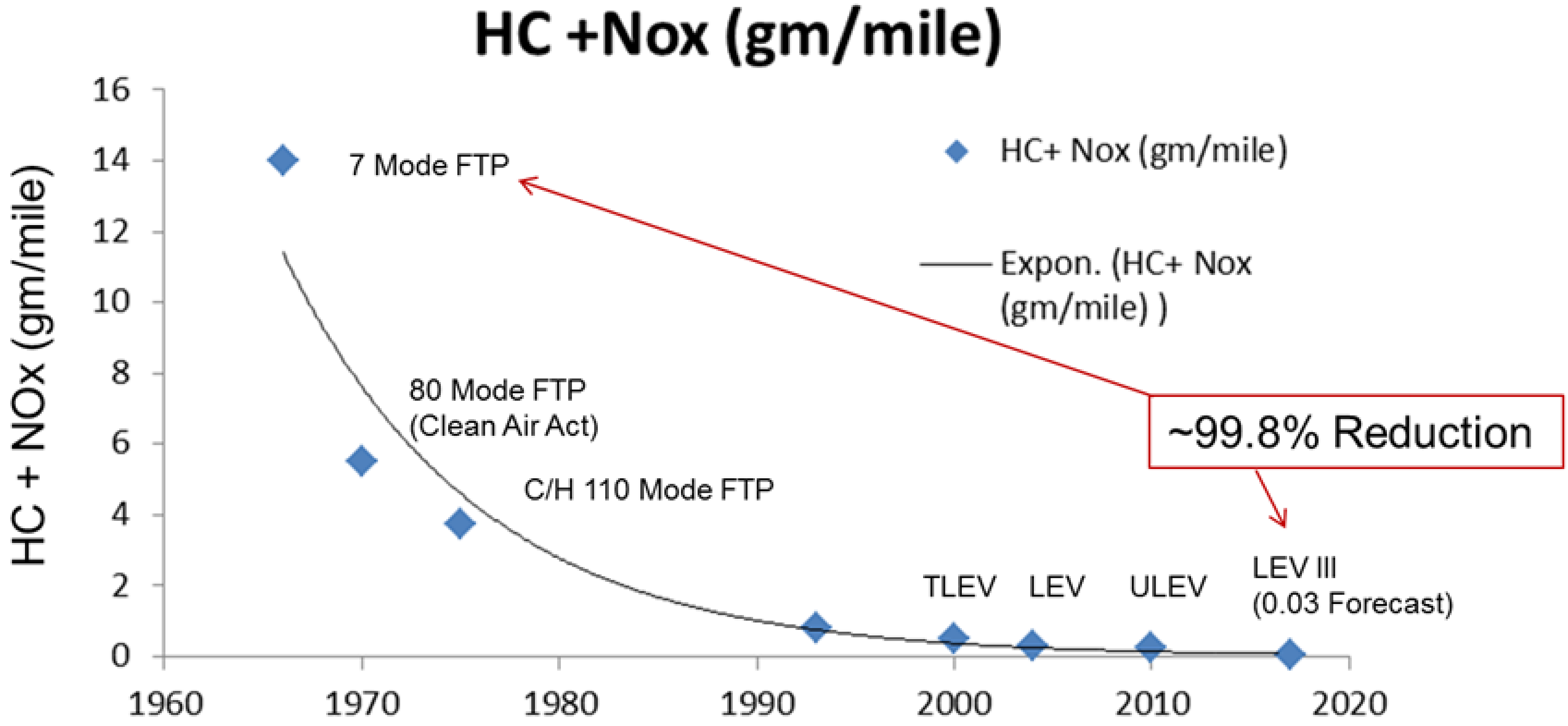
benzene, 1,3-butadiene, formaldehyde, acrolein, acetaldehyde,
and diesel particulate matter (DPM).

Harmful effects on the central nervous system:

BTEX/N/S - benzene, toluene, ethylbenzene, xylenes, Naphthalene, Styrene

Engine emissions - transportation & toxic air pollutants

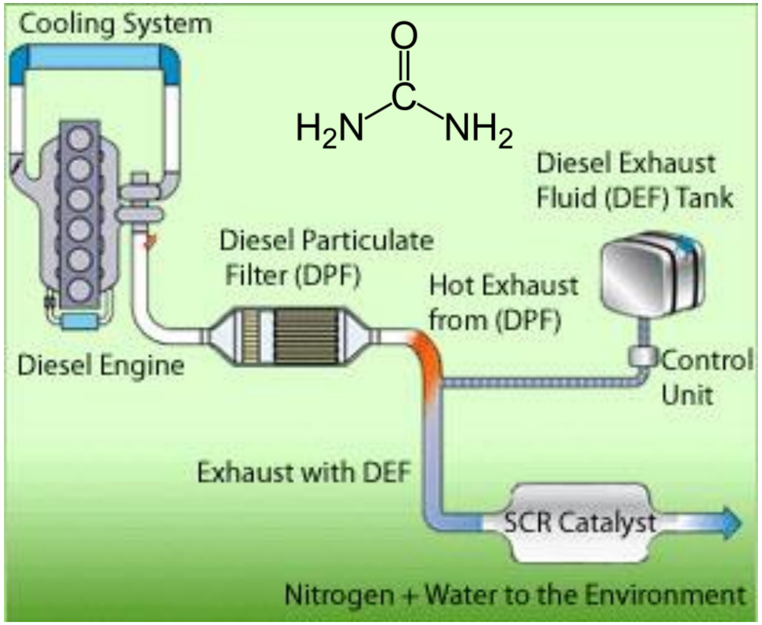
Future emissions standards will be a challenging constraint.



Diesel emission solutions

– Selective Catalytic Reduction (SCR) and Diesel Particulate Filter (DPF)

US EPA 2010 HD soot: 0.0134 g/kW-hr
NOx: 0.2682 g/kW-hr.



1.) <u>EGR?</u>

Navistar – no SCR

<u>Enabling technologies</u> (Cost?):

Improved combustion bowl design - PCCI
Improved EGR valves, air-handling, VVA
Twin-series turbochargers, inter-stage cooling
High-pressure CR fuel injection (31,800 psi)

2.) <u>SCR?</u>

Cummins Cu-Zeolite with DEF for 2010
Claim 3-5% fuel economy gain (Class 8 truck 1% ≈$1,000 per year)
“StableGuard Premix” dose rate ~2% of fuel consumption rate
Cost? $3/gal? AdBlue at pump in Germany $12/gal
Volvo announced surcharge of $9,600 for 2010 compliance
(complex – dosing rate, DEF freezes at 12F, gasifies at 130F)
Plus $7,500 for 2007 compliance → <u>AT system cost equals cost of engine!</u>

Yoshikawa, 2008

NOx modeling

Zeldo’vich thermal NOx mechanism

$O + N_2 <=> NO + N$ ← Rate controlling step due to high N_2 bond strength

$N + O_2 <=> NO + O$

$N + OH <=> NO + H$

ERC 12-step NOx model is based on GRI-Mech v3.11 and includes:

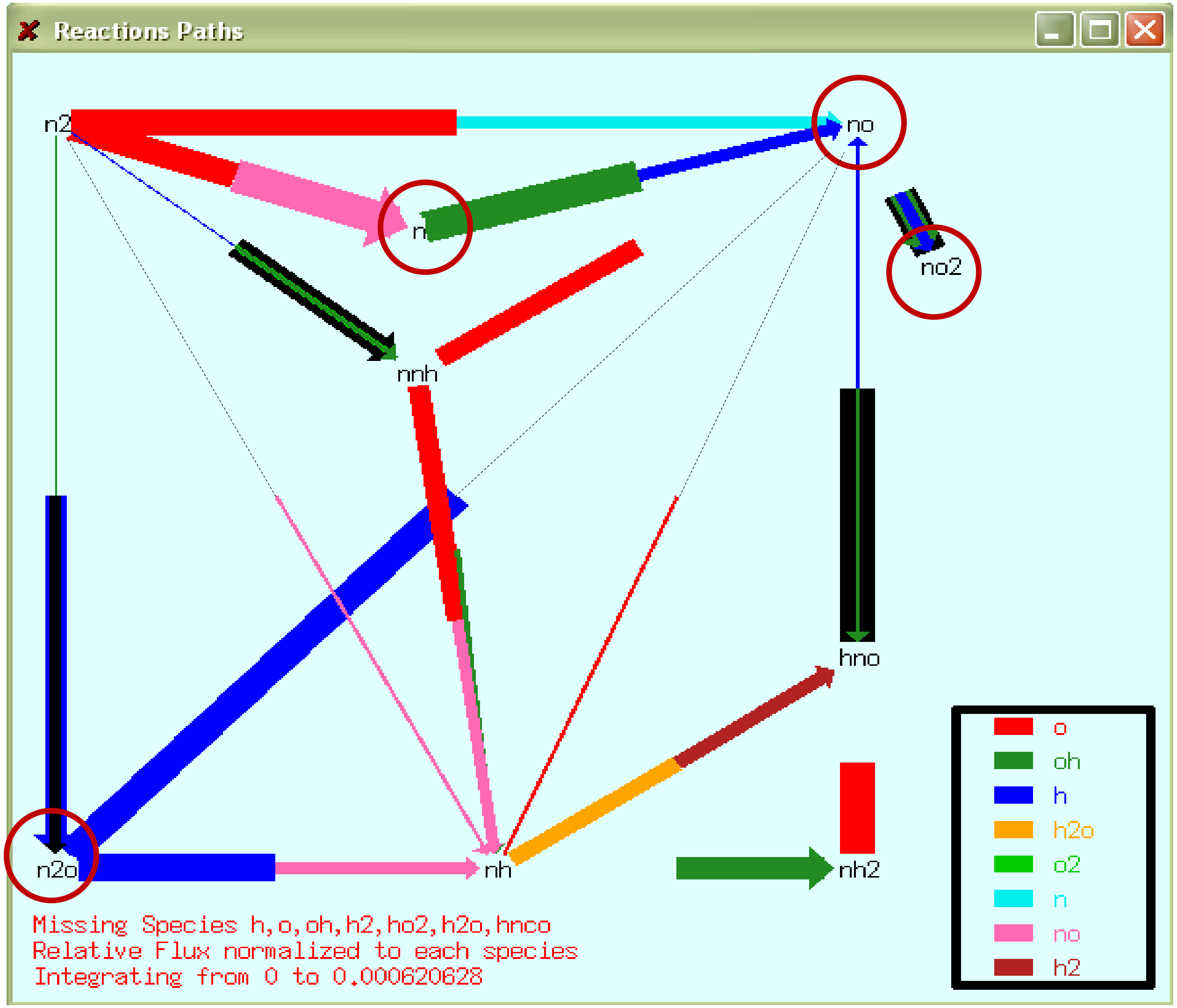
- Thermal NOx — Zeldovich, 1946
- Prompt NOx around 1000 K. — Fenimore, 1979

Extensions

- NO can convert HCN and NH_3 — Eberius, 1987
- Interaction between NO and Soot — Guo, 2007

Kong, 2007

ERC 12 step NOx Mechanism



Missing Species h,o,oh,h2,ho2,h2o,hnco
Relative Flux normalized to each species
Integrating from 0 to 0.000620628

SENKIN2 used to predict species histories.

XSENKPLOT used to visualize reaction pathways and identify important reactions and species.

Reduced mechanism validated for test temperatures from 700K to 1100 K and equivalence ratios from 0.3 to 3.0.

Four additional species (N, NO, N_2O, NO_2) and 12 reactions added to ERC PRF mechanism

Detailed mechanism: Smith, GRI-mech, 2005

Kong, 2007

ERC 12 step NOx mechanism

Diesel spray computations

$N + NO <=> N_2 + O$

$N + O_2 <=> NO + O$

$N + OH <=> NO + H$

$N_2O + O <=> N_2 + O_2$

$N_2O + O <=> 2NO$

$N_2O + H <=> N_2 + OH$

$N_2O + OH <=> N_2 + HO_2$

$N_2O + M <=> N_2 + O + M$

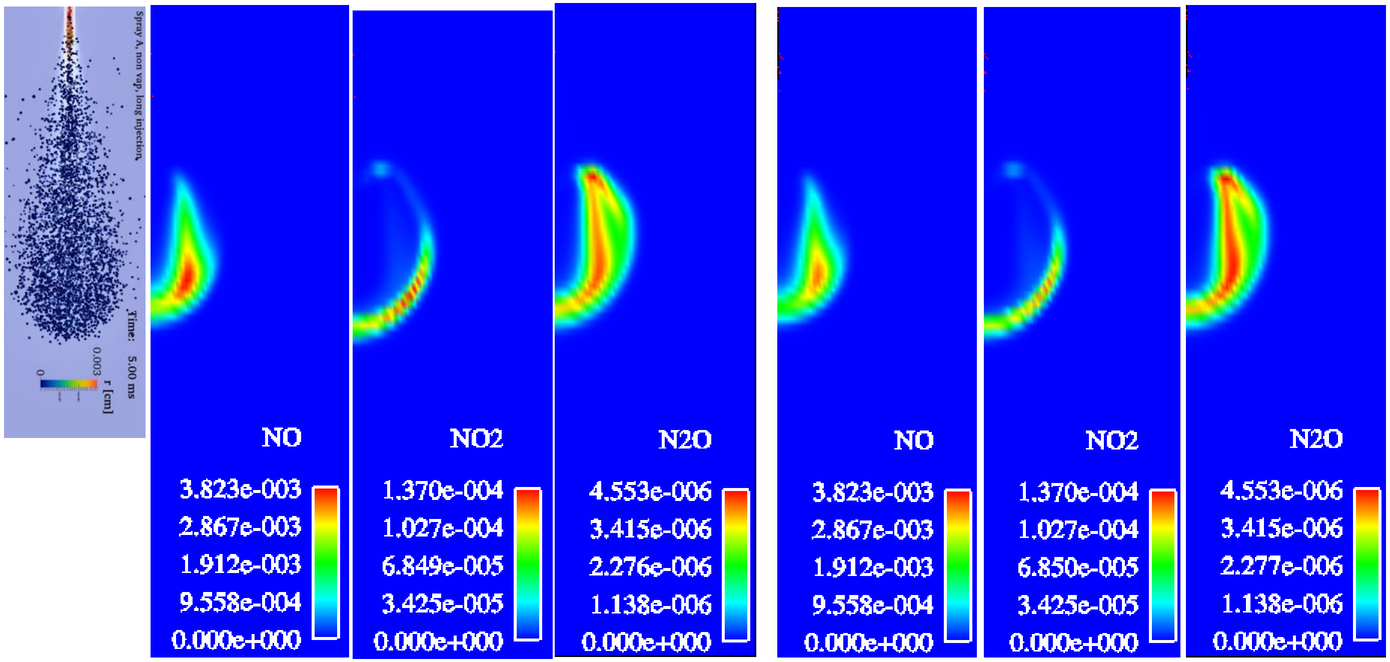
$HO_2 + NO <=> NO_2 + OH$

$NO + O + M <=> NO_2 + M$

$NO_2 + O <=> NO + O_2$

$NO_2 + H <=> NO + OH$

Comparison of NOx predictions (T=900K, P=3.7MPa)



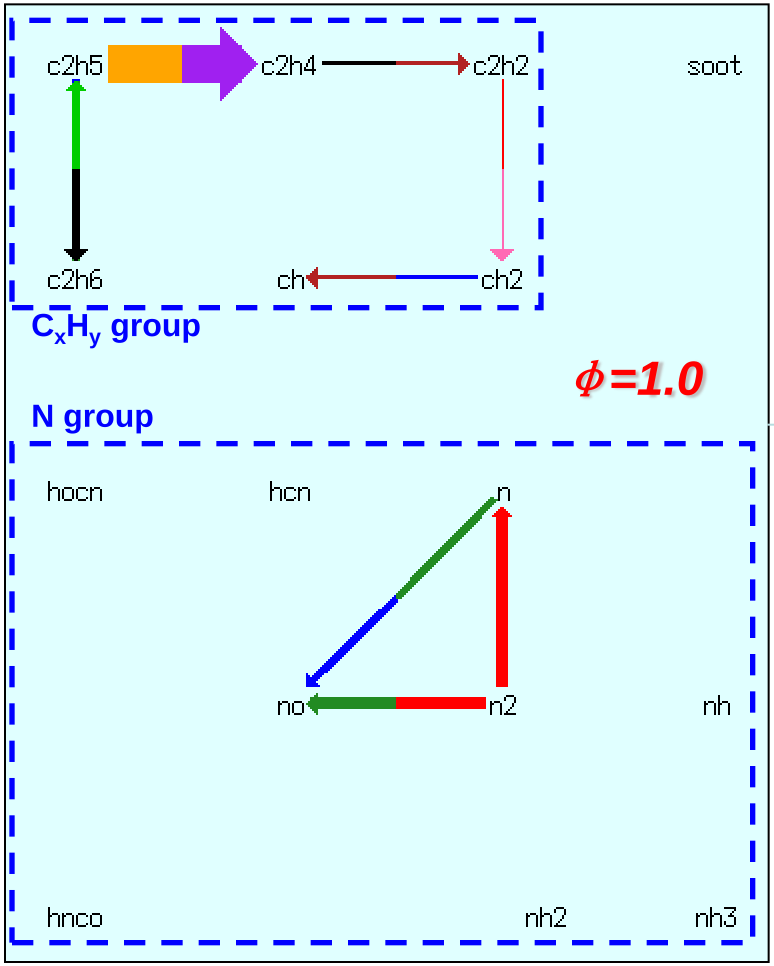
GRI mechanism results

Reduced mechanism results

Detailed mechanism: Smith, GRI-mech, 2005

Yoshikawa, 2008

CH radical and HCN bridge in fuel-rich regions



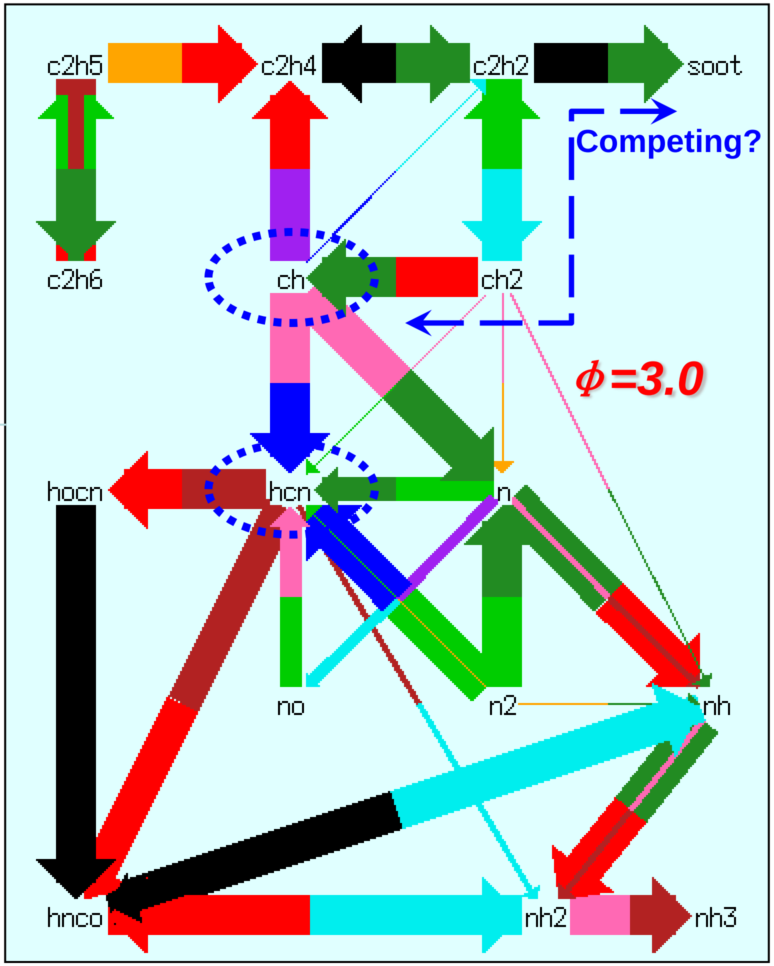
Constant volume SENKIN analysis with ERC n-heptane mechanism & GRI ver.3 NOx mechanism

Absolute Flux normalized to NO by XSENKPLOT

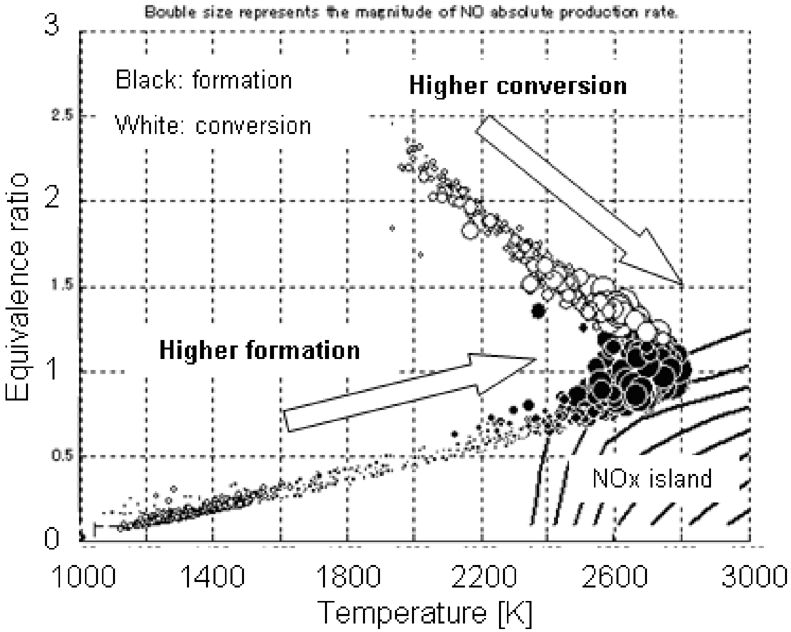
T_{ini}=769K

P_{ini}=40bar

Time=100ms



Influence of soot radiation on combustion and NOx

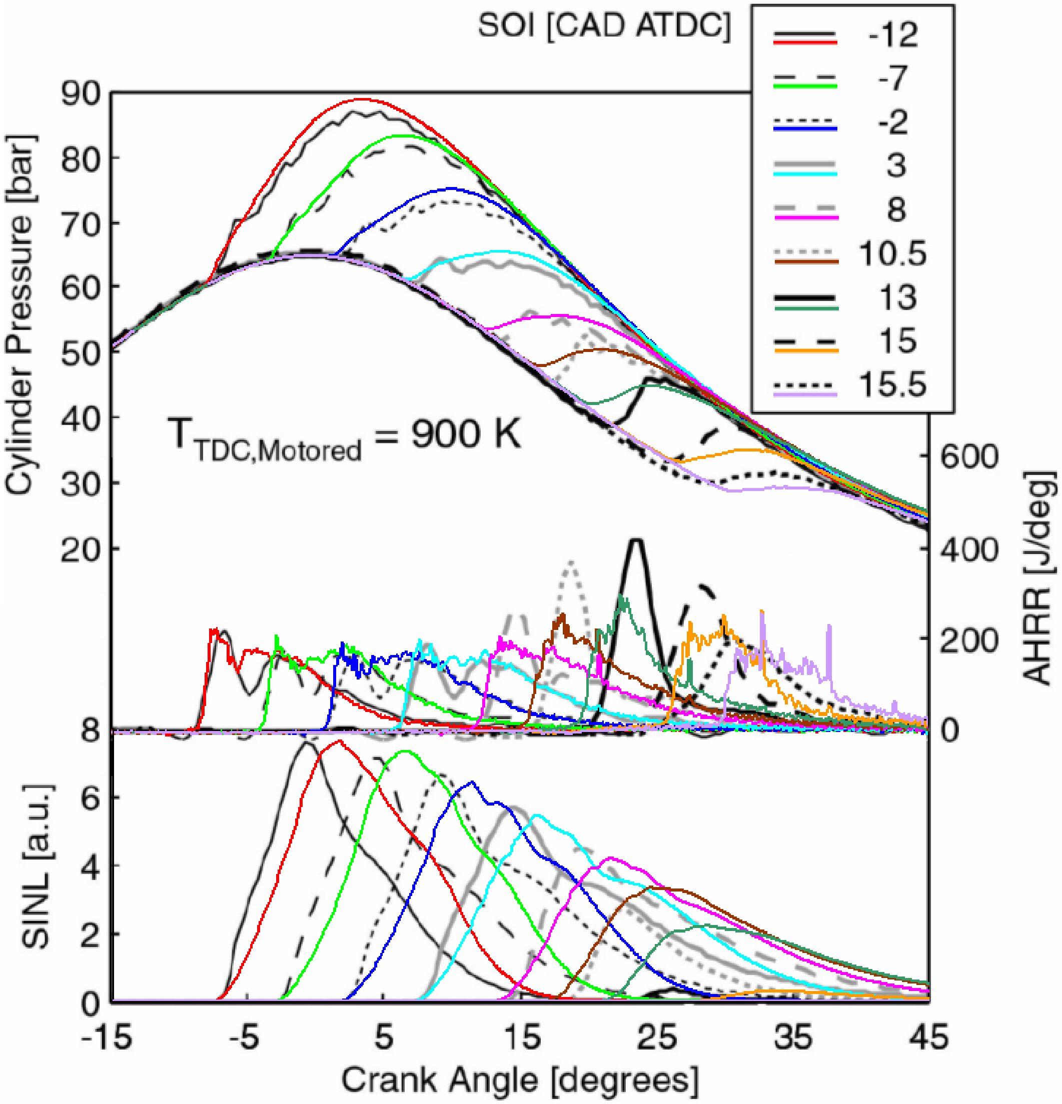


BW: measured

Musculus, 2005

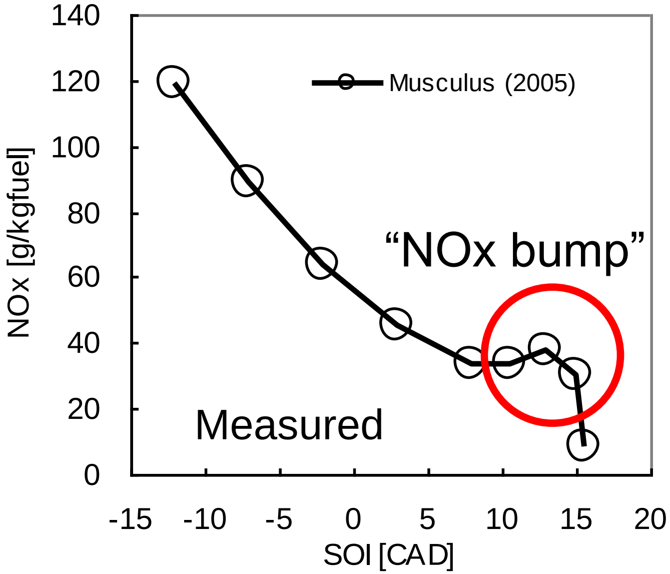
Colored: prediction

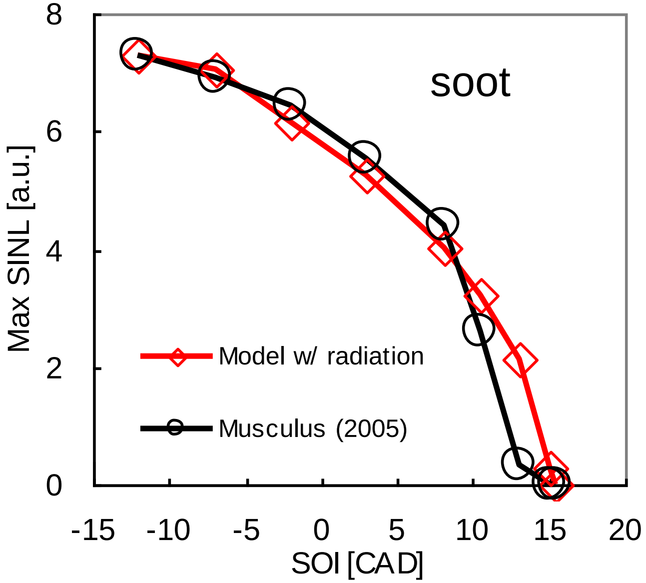
Yoshikawa, 2009

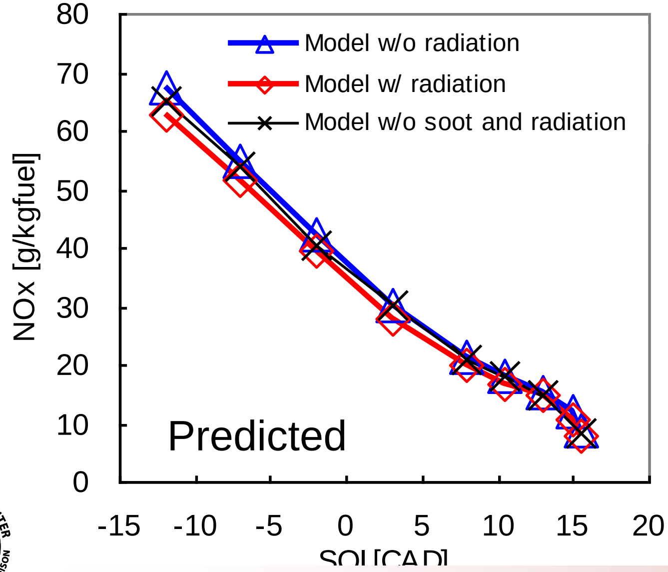


Yoshikawa, 2009

Influence of soot radiation on combustion and NOx







"NOx bump" not observed in prediction, but reduction in predicted NOx seen with retard of SOI (~ SOI=8 CAD ATDC)

Radiation lowers predicted NOx ~ 7.5 %

Absence of soot lowered predicted NOx ~ 2.5 %

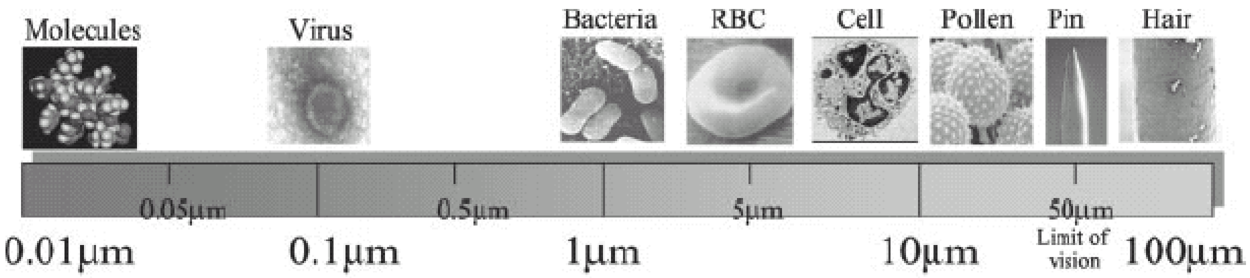
NOx model underpredicts measured NOx

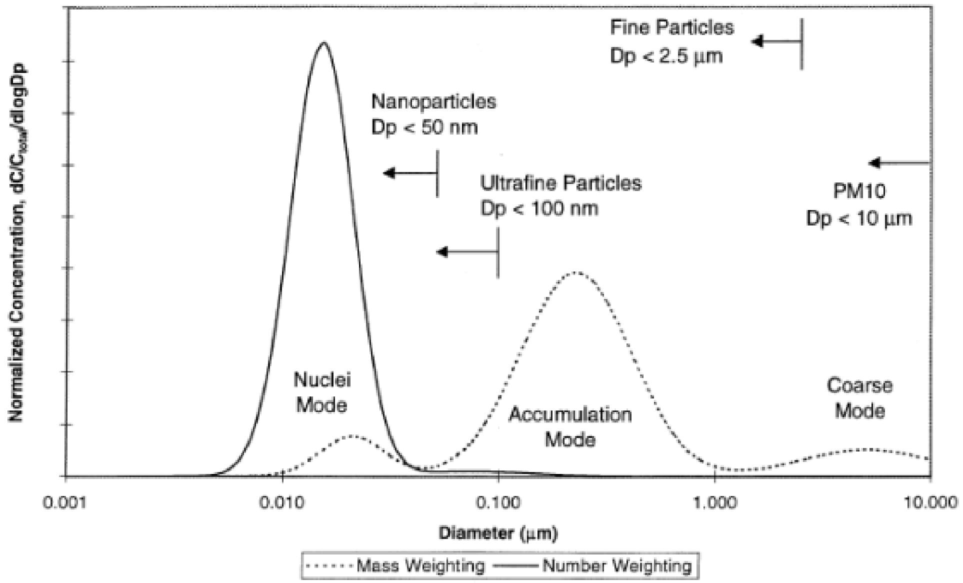
Magnitude sensitive to turbulent Schmidt #

Kittelson, 1998

Particulate emissions

Regulated emissions PM2.5





New challenge - engines must meet particulate number-based regulations (PN).

Euro 6:

PN limit 6.0e11 particles/km for vehicles produced after 2017.

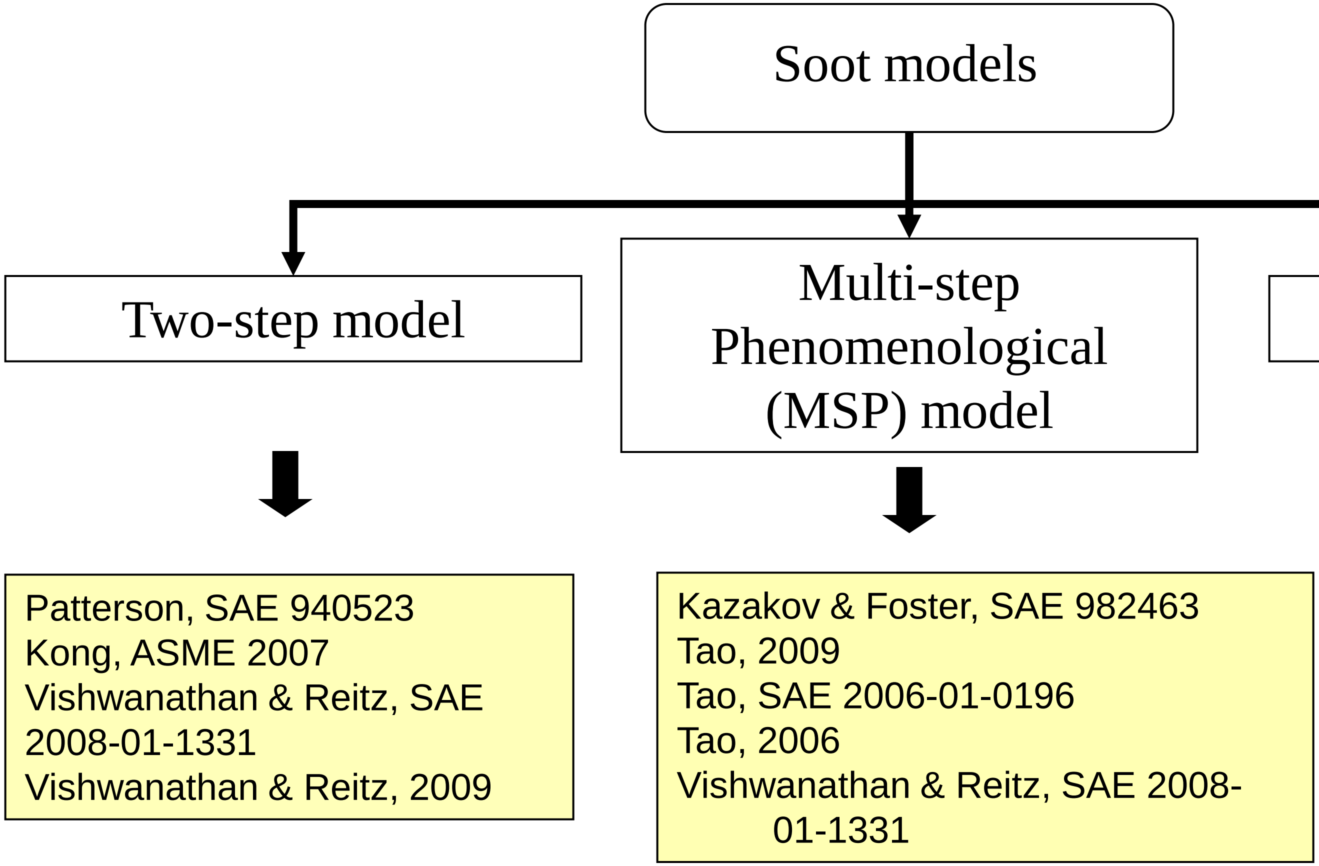
California Air Resources Board (CARB) LEV III:

Total PM mass: 3.8 mg/km for 2014 and 1.9mg/km for 2017

PN: 3.8e12 and 1.9e12 particle/km.

Greatest health risk - fine particles can lodge deeply into the lungs

Soot modeling at the ERC



Soot models

Two-step model

Multi-step Phenomenological (MSP) model

PAH chemistry

Patterson, SAE 940523
Kong, ASME 2007
Vishwanathan & Reitz, SAE 2008-01-1331
Vishwanathan & Reitz, 2009

Kazakov & Foster, SAE 982463
Tao, 2009
Tao, SAE 2006-01-0196
Tao, 2006
Vishwanathan & Reitz, SAE 2008-01-1331

Vishwanathan & Reitz, CST 2010

Models of soot formation/oxidation – Kennedy, Prog. Energy Comb. Sc., 1997
Soot processes in engines - Tree and Svenson, Prog. Energy Comb. Sc., V2007

Two-step model

Hiroyasu soot formation

"tuning" constant

$$\dot{M}_{sf} = \boxed{A_{sf}} \cdot P^{0.5} \cdot \exp(-E_{sf}/RT) \cdot M_{C2H2}$$

Nagle and Strickland-Constable (NSC) oxidation

$$\dot{M}_{so} = \frac{6}{\rho_s D_{nom}} \cdot W_{nsc} \cdot M_s$$

Net soot mass

$$\frac{d(M_s)}{dt} = \dot{M}_{sf} - \dot{M}_{so}$$

C_2H_2 soot precursor

ρ_s = Soot density = 2 g/cm^3

D_{nom} = assumed nominal soot diameter

= 25 nm

W_{nsc} = NSC oxidation rate/area

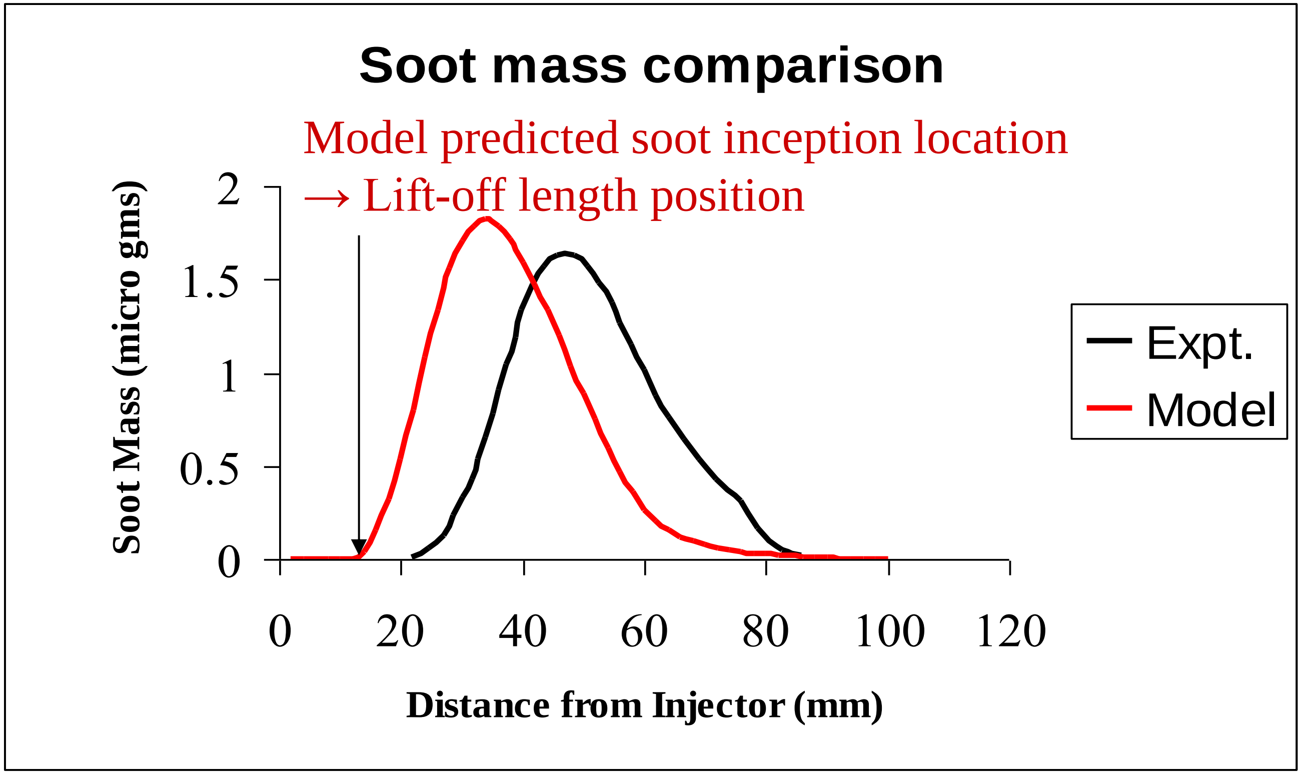
M_{c2h2} = C_2H_2 Mass, M_s = Mass of soot

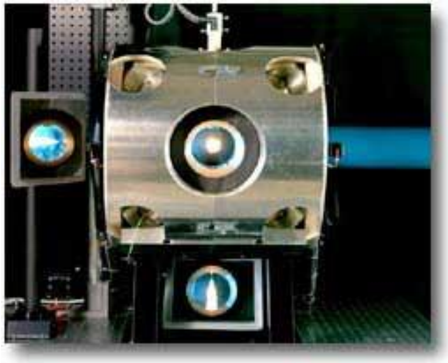
Hiroyasu & Kadota, SAE 760129
Nagle & Strickland-Constable, 1962

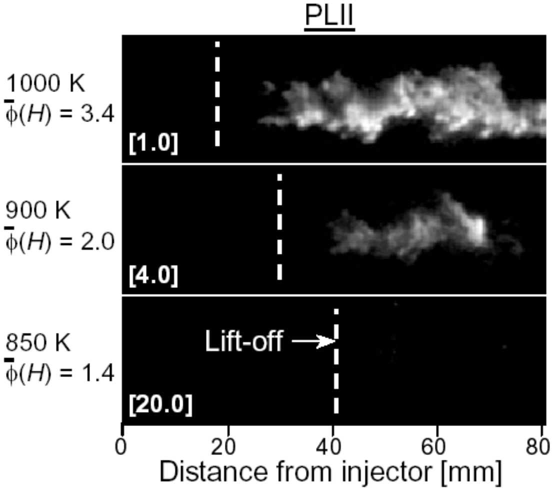
Vishwanathan, 2008

Performance of two-step soot model

SANDIA spray chamber: Pickett, 2004





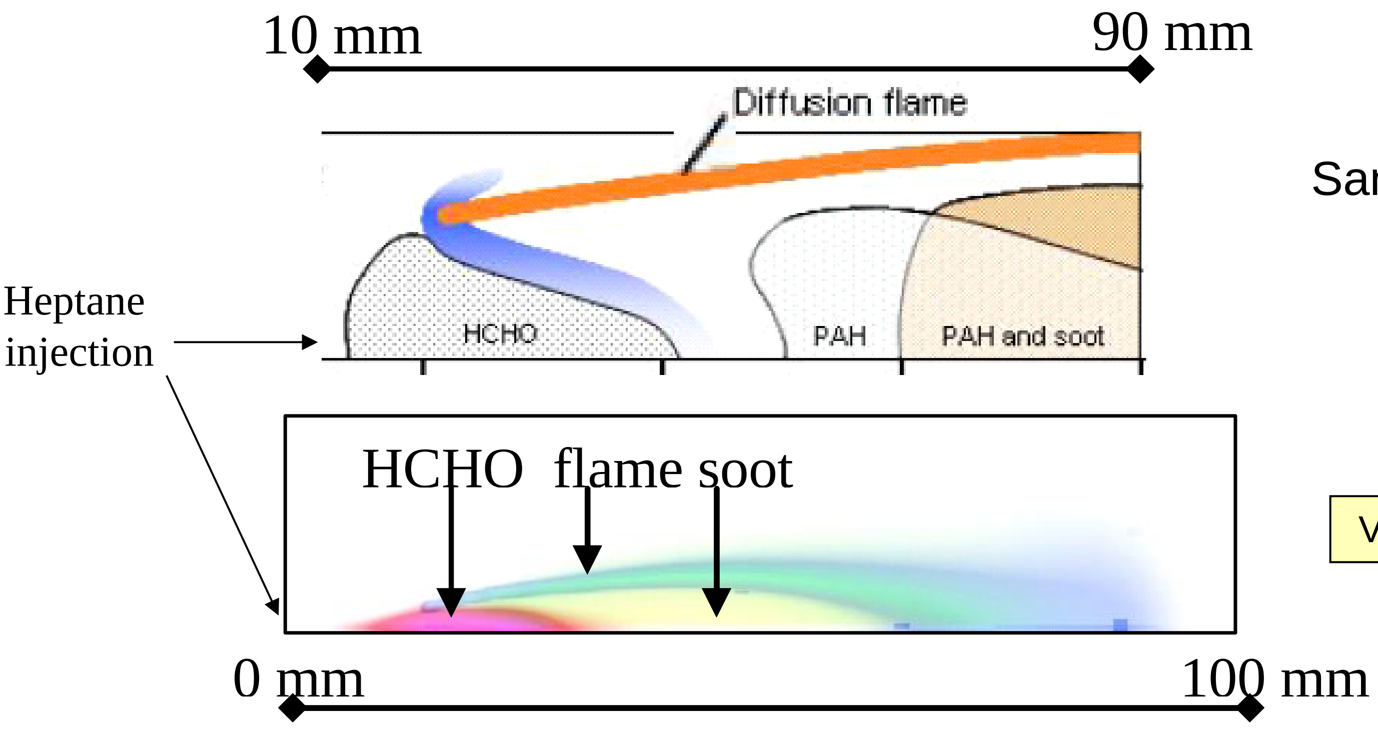


C_2H_2 inception occurs at lift-off location

Inclusion of PAH chemistry needed for accurate prediction of soot form/oxid.

Vishwanathan, 2008

Performance of two-step soot model



Sandia experiment

Pickett, 2004

Model

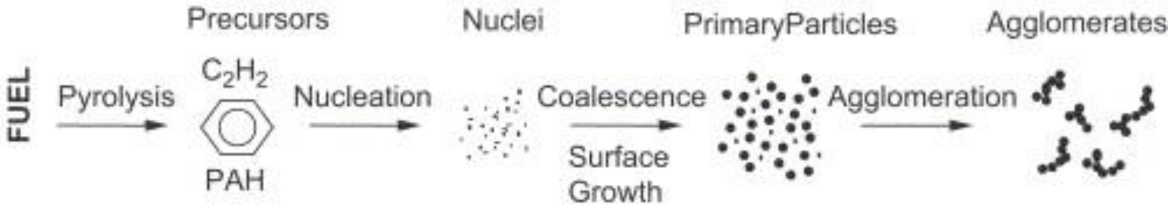
Vishwanathan, 2008

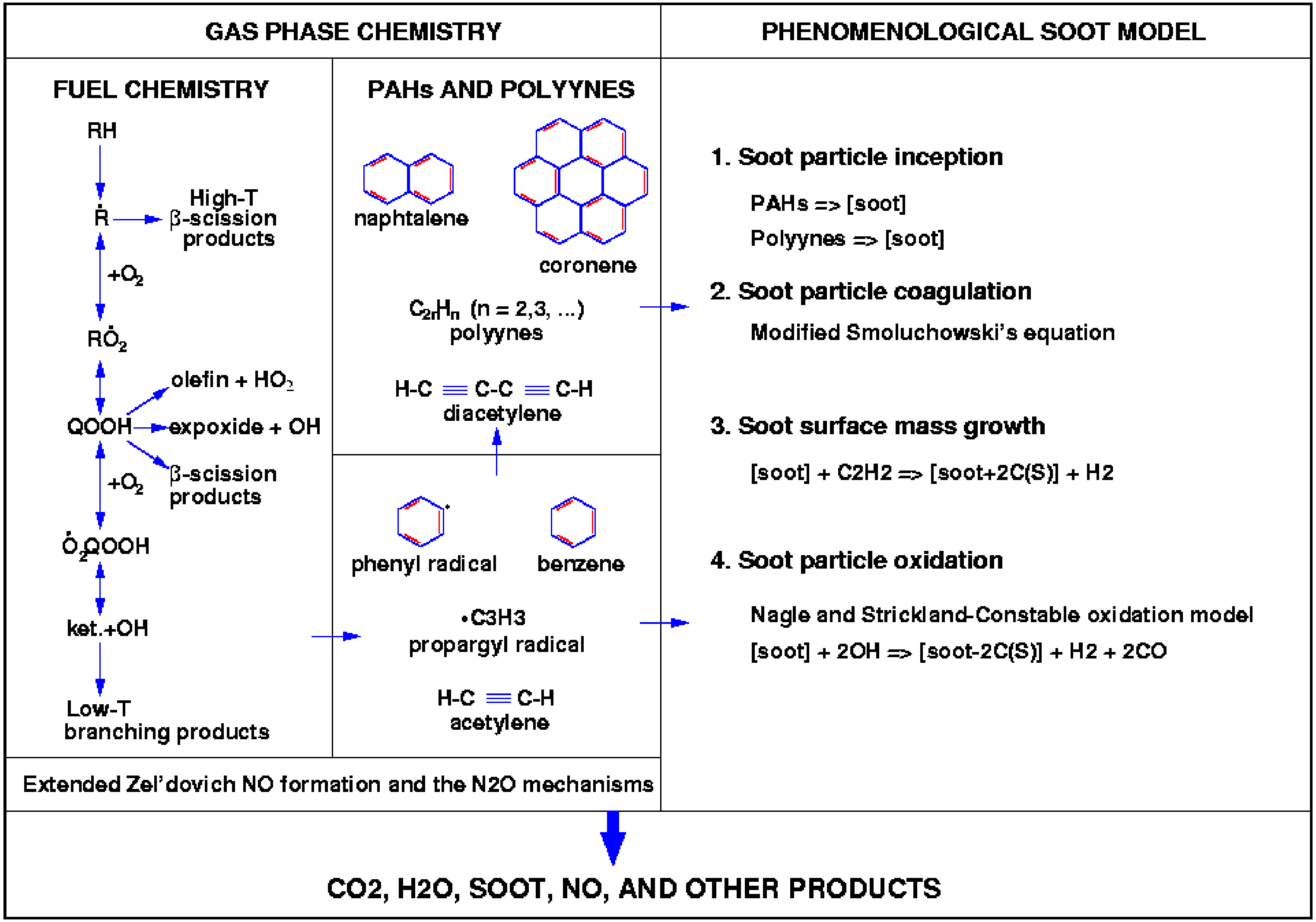
C_2H_2 inception occurs at lift-off location

Inclusion of PAH chemistry needed for accurate prediction of soot form/oxid.

Part 4: Heat transfer, NOx and Soot Emissions

Phenomenological soot models





GAS PHASE CHEMISTRY

FUEL CHEMISTRY

RH

Ṙ → High-T β-scission products

$+O_2$

$R\dot{O}_2$

QOOH → olefin + HO_2

QOOH → expoxide + OH

QOOH → β-scission products

$+O_2$

$\dot{O}_2QOOH$

ket.+OH

Low-T branching products

PAHs AND POLYYNES

naphtalene

coronene

$C_{2n}H_n$ (n = 2,3, ...) polyynes

H-C ≡ C-C ≡ C-H diacetylene

phenyl radical

benzene

•C3H3 propargyl radical

H-C ≡ C-H acetylene

Extended Zel'dovich NO formation and the N2O mechanisms

PHENOMENOLOGICAL SOOT MODEL

1. Soot particle inception

PAHs => [soot]

Polyynes => [soot]

2. Soot particle coagulation

Modified Smoluchowski's equation

3. Soot surface mass growth

[soot] + C2H2 => [soot+2C(S)] + H2

4. Soot particle oxidation

Nagle and Strickland-Constable oxidation model

[soot] + 2OH => [soot-2C(S)] + H2 + 2CO

CO2, H2O, SOOT, NO, AND OTHER PRODUCTS

Vishwanathan, 2009

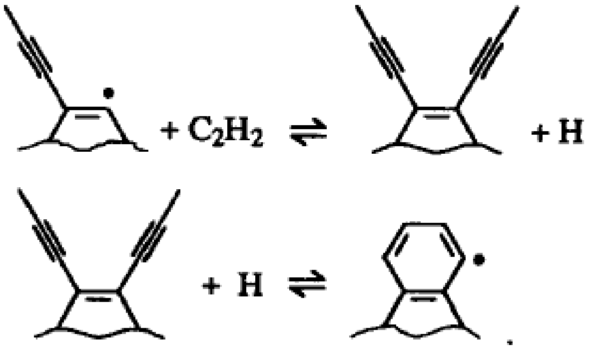
Reduced PAH mechanism

Reduced PAH mechanism of Xi & Zhong, 2006 based on detailed mechanism of Wang &Frenklach, 1997 was integrated (**20 species and 52 reactions**)

A_1 formation through propargyl radical (C_3H_3)

Higher aromatics formed through HACA scheme

(hydrogen abstraction, carbon addition)



Reaction	Arrhenius parameters-A, n, E. (Units of A in mole-cm-sec-K and units of E in cal/mole)
$C_3H_3 + C_3H_3 \rightarrow A_1$	2.0E+12, 0.0, 0.0
A_1- + $C_4H_4 \leftrightarrow A_2$ + H	2.50E+29, -4.4, 26400.0
A_1+ A_1-↔ P_2 + H	1.10E+23, -2.9, 15890.0
A_2-1 + $C_4H_4 \leftrightarrow A_3$ + H	2.50E+29, -4.4, 26400.0
$A_1C_2H^*$ + $A_1 \leftrightarrow A_3$ + H	1.10E+23, -2.9, 15890.0
A_3-4 + $C_2H_2 \leftrightarrow A_4$ + H	3.00E+26, -3.6, 22700.0

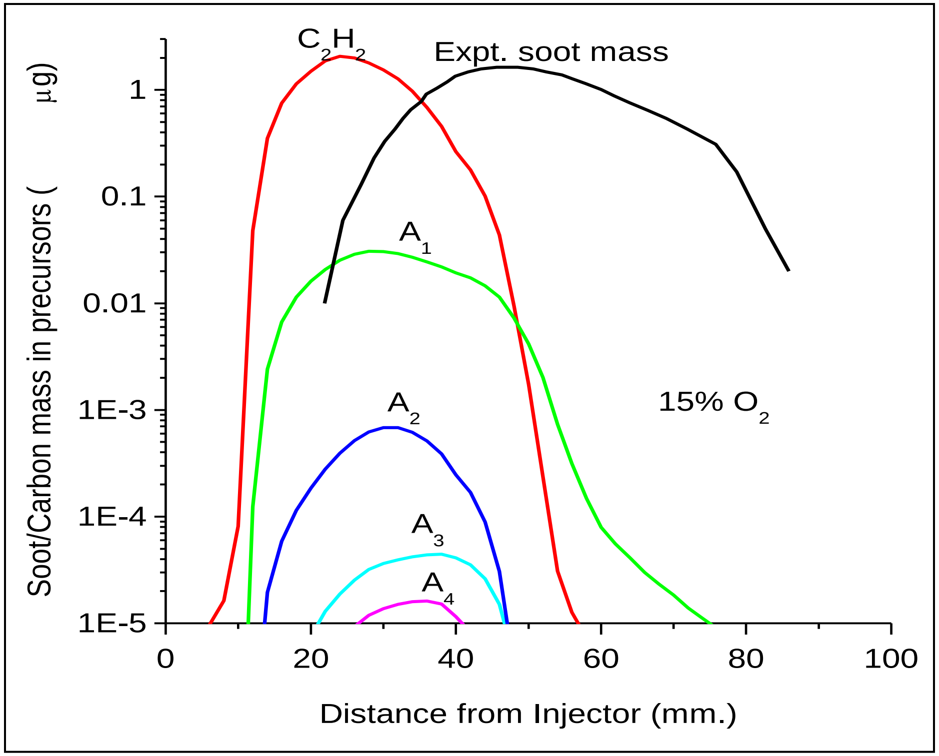
A_1 = benzene, A_2 = naphthalene, P_2 = biphenyl, A_3 = phenanthrene, A_4= pyrene, A_1- = phenyl, A_2-1 = 1-naphthyl, A_3-4 = 4-phenanthryl, $A_1C_2H^*$ = phenylacetylene radical

Vishwanathan, 2009

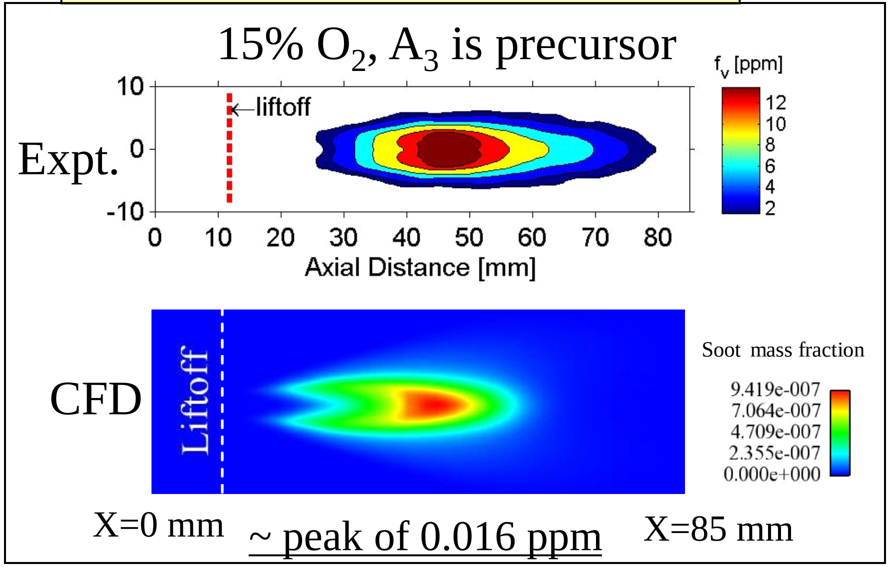
PAH species

Reduced PAH mechanism implemented considering up to 4 aromatic rings (pyrene)

- A_3 (Phenanthrene) used as precursor for soot formation model



Sandia expts: Pickett & Idicheria, 2006



Improvement in soot location

Amount of dry-carbon mass locked-up in aromatic precursors small compared to measured soot

Vishwanathan, 2010

Soot model implementation

1. Soot inception through A_4: $C_{16}H_{10}\ (A_4) \xrightarrow{\dot{\omega}_1} 16C(s) + 5H_2$ ⟶ Graphitization

$$\dot{\omega}_1 = k_1 \cdot [A_4],\ k_1 = 2000\ \{s^{-1}\}$$

2. C_2H_2 assisted surface growth: Leung, 1991 $C(s) + C_2H_2 \xrightarrow{\dot{\omega}_2} 3C(s) + H_2$

$$\dot{\omega}_2 = k_2 \cdot [C_2H_2],\ k_2 = 9.0 \cdot 10^4 \exp(-12100/T) \cdot \sqrt{S}\ \ \{s^{-1}\}$$

$$S = \pi d_p^2 N\ \ \{cm^{-1}\}$$ ⟶ Surface area per unit volume

$$d_p = \left(\frac{6\boxed{Y_{c(s)}\rho}}{\pi\rho_{c(s)}\boxed{N}}\right)^{1/3}\ \{cm\}$$ ⟶ Particle size

$Y_{C(S)}$ = soot mass fraction

N = soot number density (per cc)

$\rho_{C(S)} = 2.0\ gm/cm^3$

$M_{C(S)}$ = MW of carbon

K_{bc} = Boltzmann's constant

C_a = agglomeration constant = 9

Mono –disperse locally: All soot in a comp. cell have same diameter

3. Soot coagulation: Leung, 1991 $nC(s) \xrightarrow{\dot{\omega}_3} C(s)_n$

$$\dot{\omega}_3 = 2C_a \left(\frac{6M_{c(s)}}{\pi\rho_{c(s)}}\right)^{1/6} \cdot \left(\frac{6K_{bc}T}{\rho_{c(s)}}\right)^{1/2} \cdot \left[\frac{\rho Y_{c(s)}}{M_{c(s)}}\right]^{1/6} \cdot [N]^{11/6}\ \ \{particles\ cm^{-3}s^{-1}\}$$

Vishwanathan, 2010

Soot model implementation

4. O_2 assisted soot oxidation (NSC model):

$$C(s) + \frac{1}{2}O_2 \xrightarrow{\dot{\omega}_4} CO$$

$$\dot{\omega}_4 = \frac{12}{M_{c(s)}} \cdot \left(\left(\frac{K_A P_{O_2}}{1+K_Z P_{O_2}} \right) \cdot x + K_B P_{O_2} \cdot (1\text{-}x) \right) \cdot S \ \{\text{mol cm}^{-3}\ \text{s}^{-1}\}$$

$$x = P_{O_2} \big/ (P_{O_2} + (K_T/K_B))$$

$$K_A = 30.0 \cdot \exp(-15800/T)\ \{\text{g cm}^{-2}\ \text{s}^{-1}\ \text{atm}^{-1}\}$$

$$K_B = 8.0 \cdot 10^{-3} \cdot \exp(-7640/T)\ \{\text{g cm}^{-2}\ \text{s}^{-1}\ \text{atm}^{-1}\}$$

$$K_T = 1.51 \cdot 10^{5} \cdot \exp(-49800/T)\ \{\text{g cm}^{-2}\ \text{s}^{-1}\}$$

$$K_Z = 27.0 \cdot \exp(3000/T)\ \{\text{atm}^{-1}\}$$

x = fraction of A sites

$(1\text{-}x)$ = fraction of B sites

P_{O2} = partial pressure of O_2

$K_{A,B,T,Z}$ = rate constants

X_{OH} = mole fraction of OH

γ_{OH} = OH collision efficiency = 0.13

Fenimore, 1967

5. OH assisted oxidation (Modified Fenimore and Jones model):

$$C(s) + OH \xrightarrow{\dot{\omega}_5} CO + \frac{1}{2}H_2$$

$$\dot{\omega}_5 = (12) \cdot 10.58 \cdot \gamma_{OH} \cdot X_{OH} \cdot T^{-1/2} \cdot S\ \{\text{mol cm}^{-3}\ \text{s}^{-1}\}$$

Soot model implementation

6. PAH-assisted surface-growth

$$C(s) + PAH_{k,j} \xrightarrow{\dot{\omega}_6} C(s+k) + \frac{j}{2} H_2, \; \dot{\omega}_6 = \gamma_{ks} \cdot \beta_{ks} \cdot \left[PAH_{k,j} \right] \cdot N$$

$$\beta_{ks} = 2.2 \cdot \sqrt{\frac{\pi \cdot K_{bc} \cdot T}{2 \cdot \mu_{i,j}}} \cdot (d_p + d_{PAH})^2 \; \{cm^3 s^{-1}\}$$

$$d_{PAH} = d_A \cdot \sqrt{\frac{2m_i}{3}}$$

k = number of carbon atoms and j = number of hydrogen atoms,

γ_{ks} = 0.3 is the collision efficiency between soot and PAH, β_{ks} = collision frequency,

d_i = collisional diameter of PAH, d_A = size of single aromatic ring = 1.393√3 Å,

$\mu_{i,j}$ = Reduced mass of colliding species = Mass of PAH,

m_i = mass of PAH expressed in terms of number of carbon atoms - k

Most models consider only mono-aromatic benzene as growth species.

Soot model implementation

7. Transport equations:

$$\frac{\partial M}{\partial t} = \underbrace{-\nabla\cdot\left(M\cdot v\right)}_{\text{convection}} + \nabla\cdot\left(\underbrace{\frac{\mu}{SC}\nabla\left(\frac{M}{\rho}\right)}_{\text{diffusion}} + \underbrace{\xi\cdot M\cdot\frac{\mu}{\rho}\frac{\nabla T}{T}}_{\text{Thermophoresis}}\right) + \underbrace{\dot{S}_M}_{\text{Source terms}} \qquad \xi = 0.75 \big/ \left(1+\frac{\pi\eta}{8}\right),\ \eta = 0.9$$

$M = \rho Y_{c(s)}$ (soot species density) and N (number density) with N being treated as **passive species**

Thermophoresis term implemented as a source term

$$\dot{S}_M = \left(16\dot{\omega}_1 + 2\dot{\omega}_2 + 6\dot{\omega}_6 - \dot{\omega}_4 - \dot{\omega}_5\right)\cdot M_{c(s)} \quad \{\text{g cm}^{-3}\ \text{s}^{-1}\}\ \text{for } \rho Y_{c(s)}$$

$$\dot{S}_M = \left(16\dot{\omega}_1\cdot\frac{M_{c(s)}}{M_{nuci}} - \dot{\omega}_3\right) \quad \{\text{particles cm}^{-3}\ \text{s}^{-1}\}\ \text{for N}$$

$$M_{nuci} = \frac{\pi}{6}\cdot d_{nuci}^3\cdot\rho_{c(s)}$$

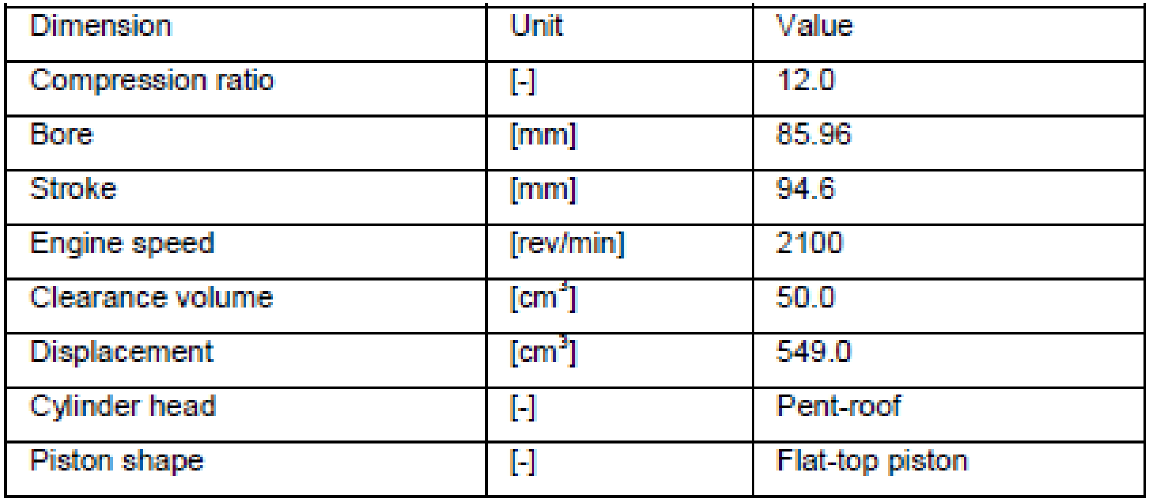
d_{nuci} = 1.25 nm (~100 carbon atoms)

Jiao, 2014

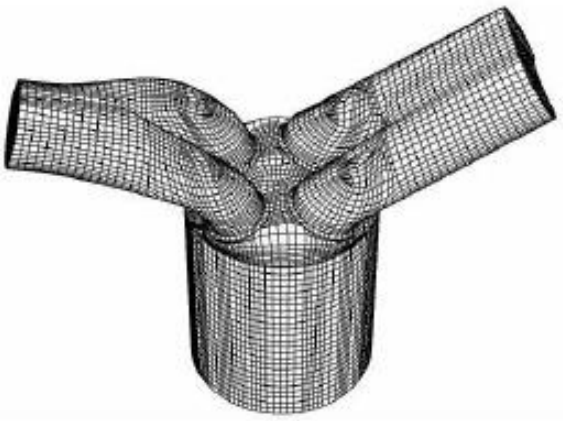
Soot mass and particle diameter prediction

Premixed charge SI engine particulate modeling

Table 1 Engine specifications.



Dimension	Unit	Value
Compression ratio	[-]	12.0
Bore	[mm]	85.96
Stroke	[mm]	94.6
Engine speed	[rev/min]	2100
Clearance volume	[cm^3]	50.0
Displacement	[cm^3]	549.0
Cylinder head	[-]	Pent-roof
Piston shape	[-]	Flat-top piston



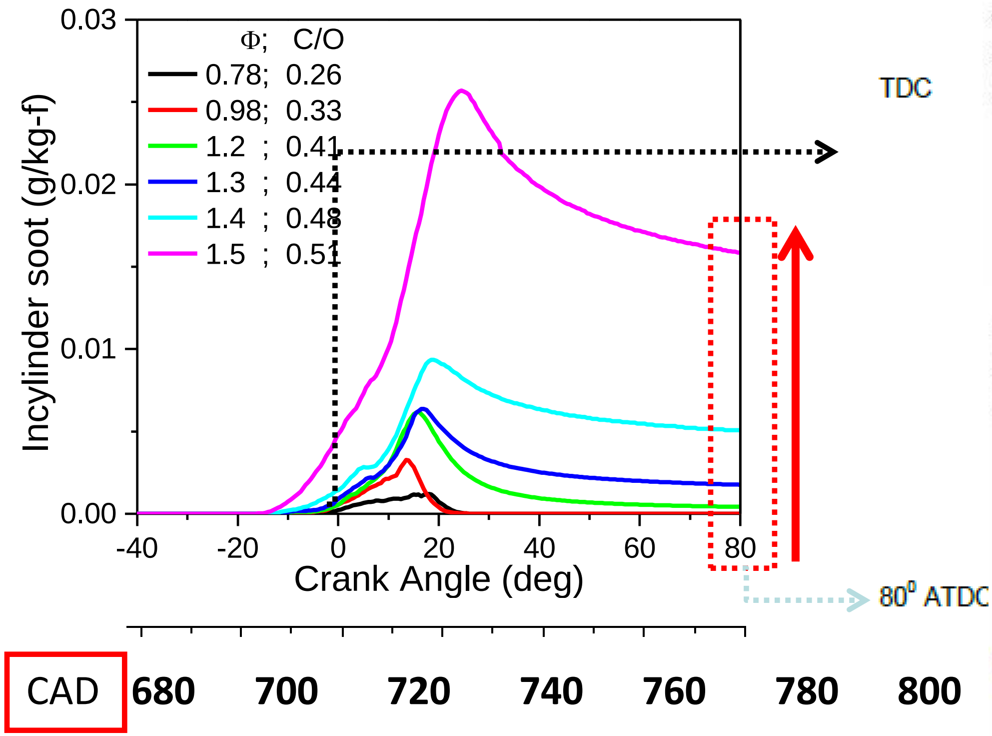
70,000 cells at BDC, including the intake and exhaust manifolds and cylinders.

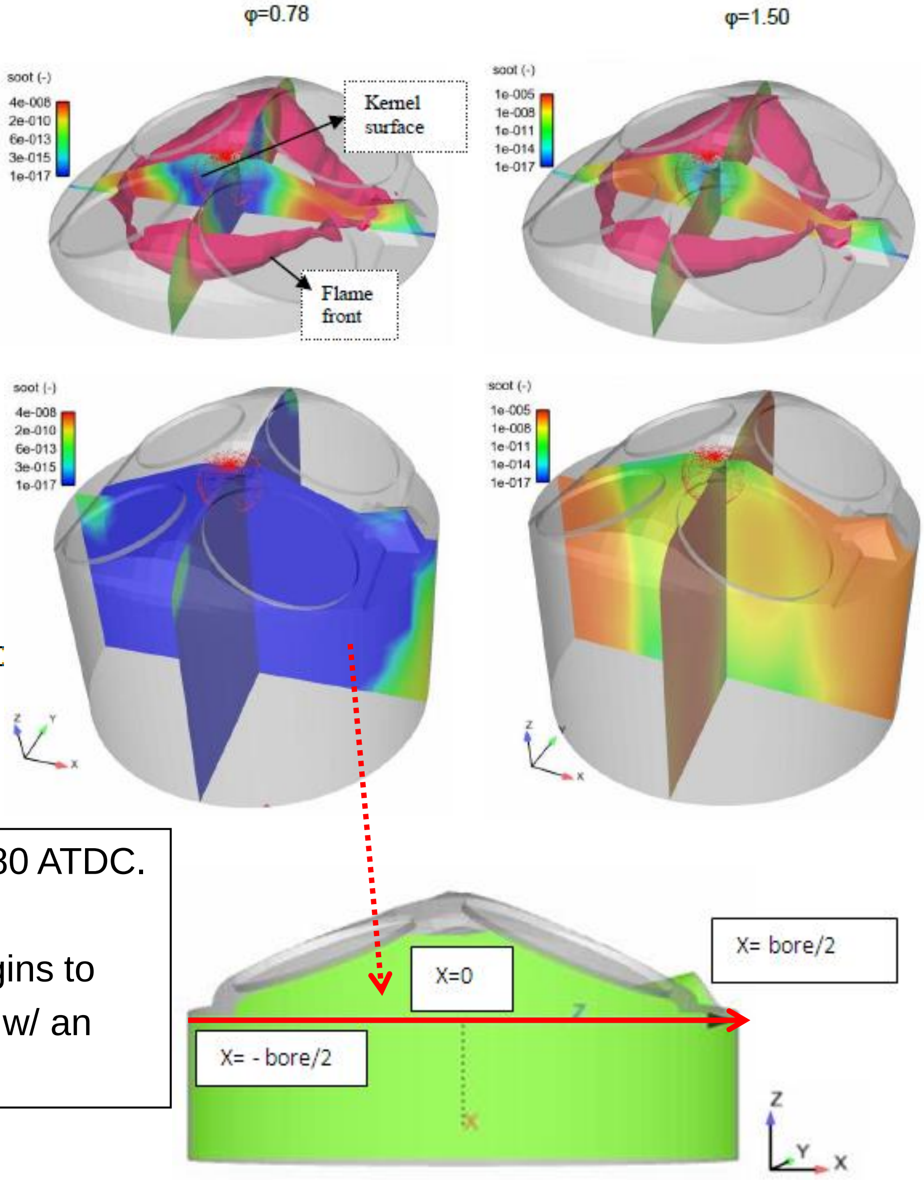
Spark plug: at center of cylinder head.
Completely homogeneous fuel/air mixture at IVC
Experiment: EPA Tier II EEE certification fuel, 28% aromatics.
ERC KIVA code simulations:
  DPIK ignition model, G-Equation combustion model.
  Fuel: iso-octane/28% toluene by volume.
  MultiChem mechanism:
    ic8h18/nc7h16/c7h8/PAH (79 species & 379 reactions)

Part 4: Heat transfer, NOx and Soot Emissions

Jiao, 2014

Soot formation prediction





Predicted soot mass no longer reduces significantly after 80 ATDC.

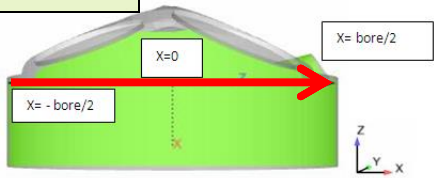
Soot produced at 80 ATDC increases with increase of φ.

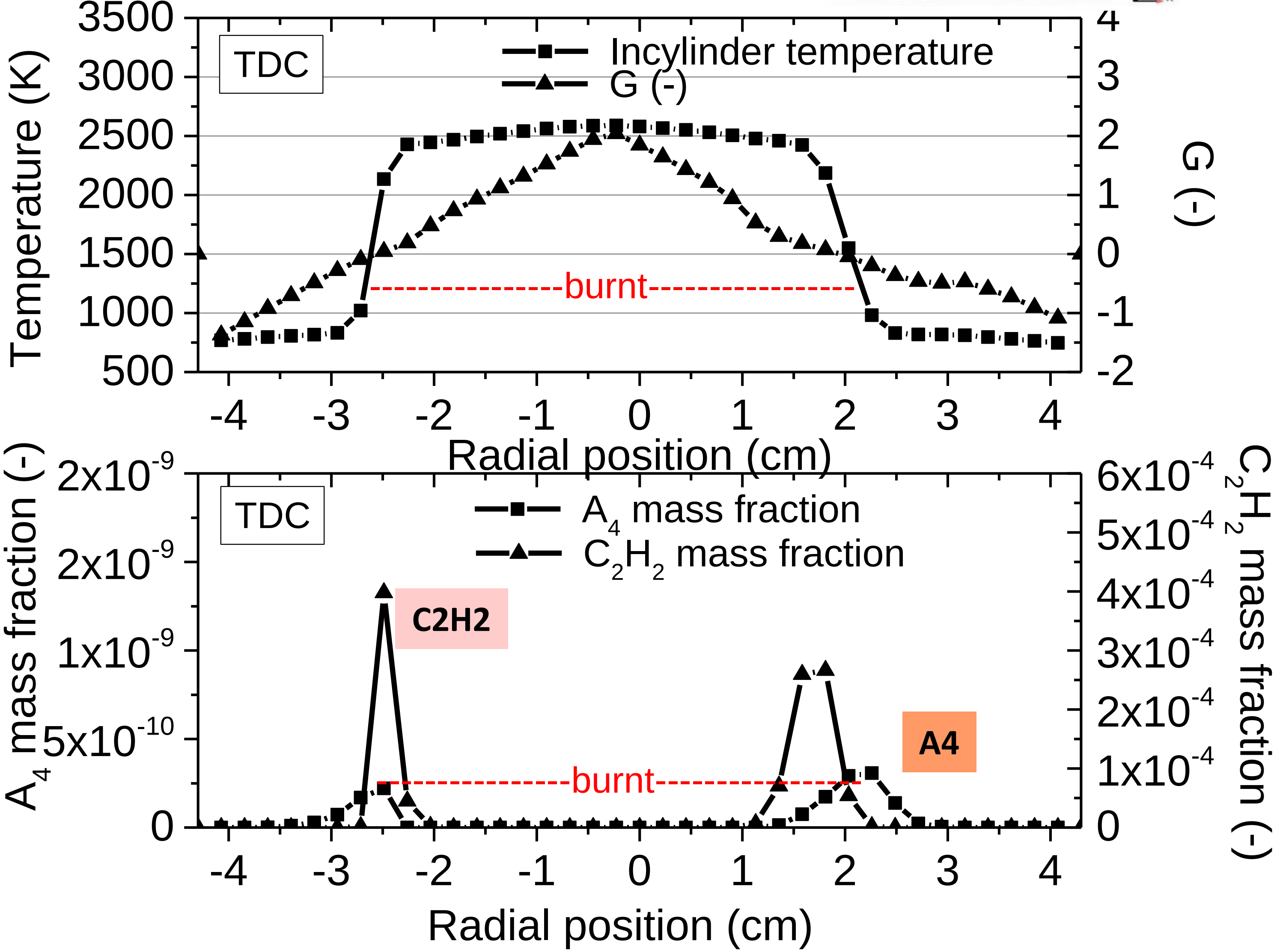
Soot formation dominates first and then soot oxidation begins to play a key role. Peak in-cylinder soot mass increases w/ an increase of φ.

Part 4: Heat transfer, NOx and Soot Emissions

Jiao, 2014

TDC ϕ =1.5

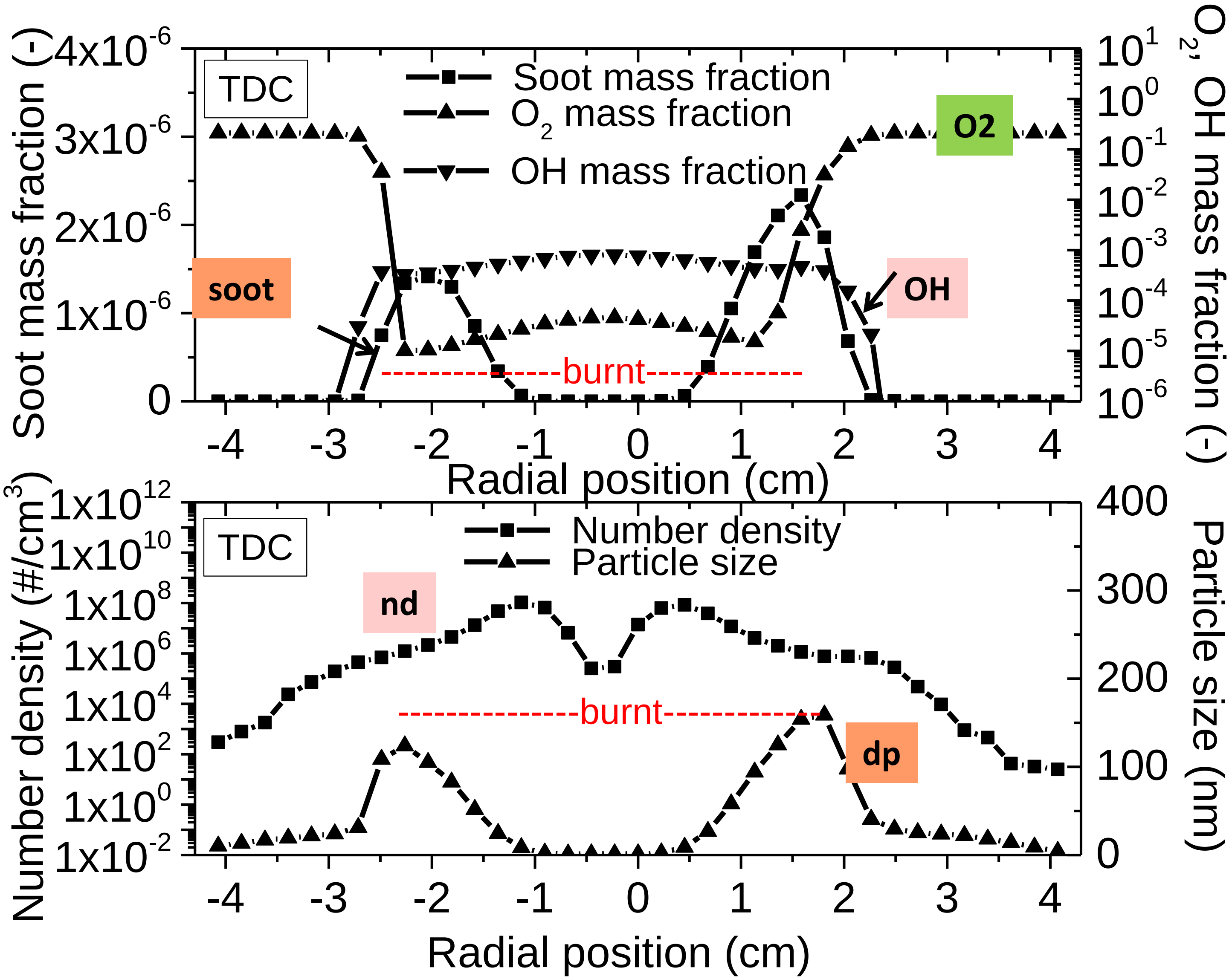




Part 4: Heat transfer, NOx and Soot Emissions

Jiao, 2014

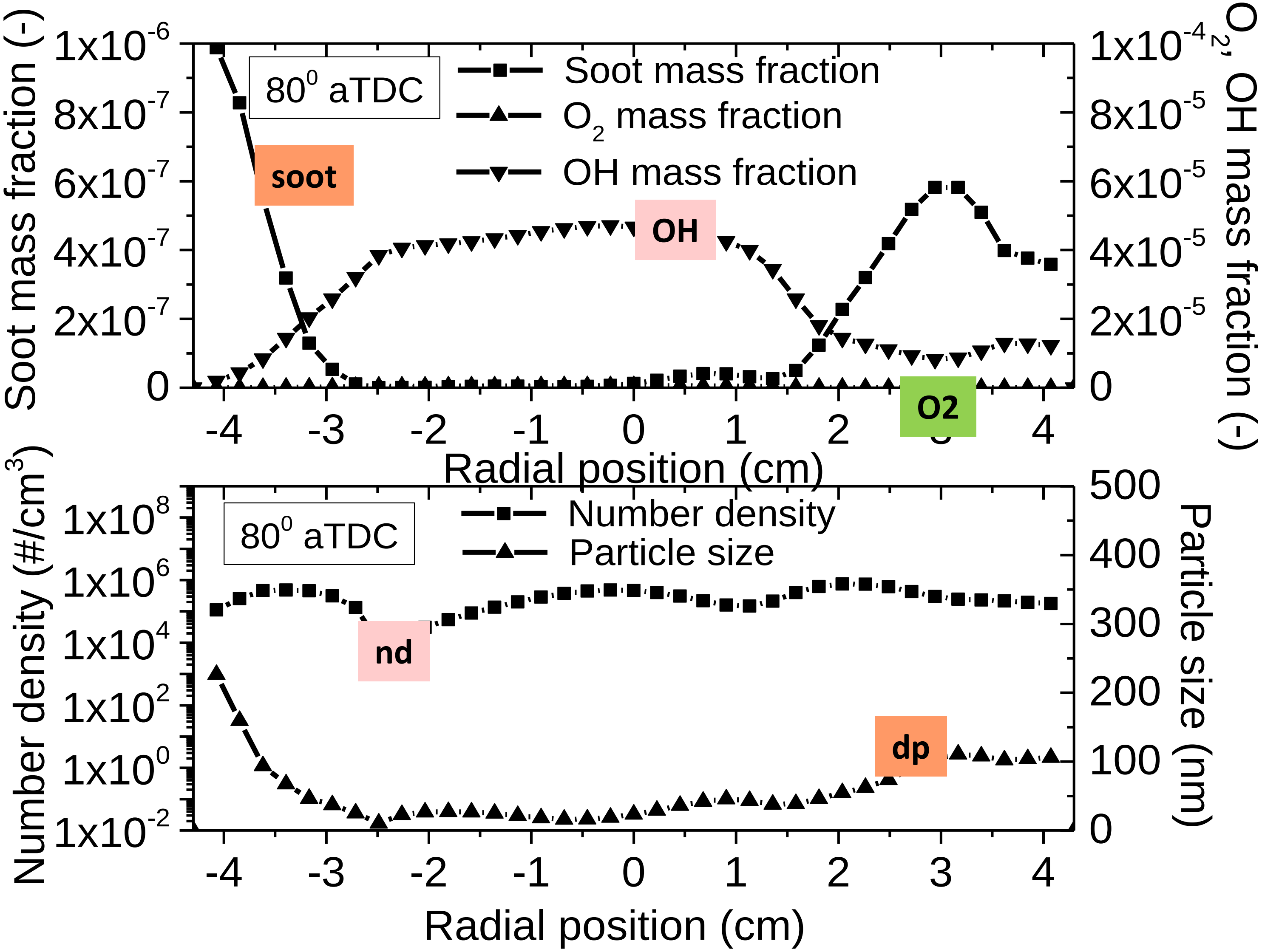
TDC ϕ =1.5



Part 4: Heat transfer, NOx and Soot Emissions

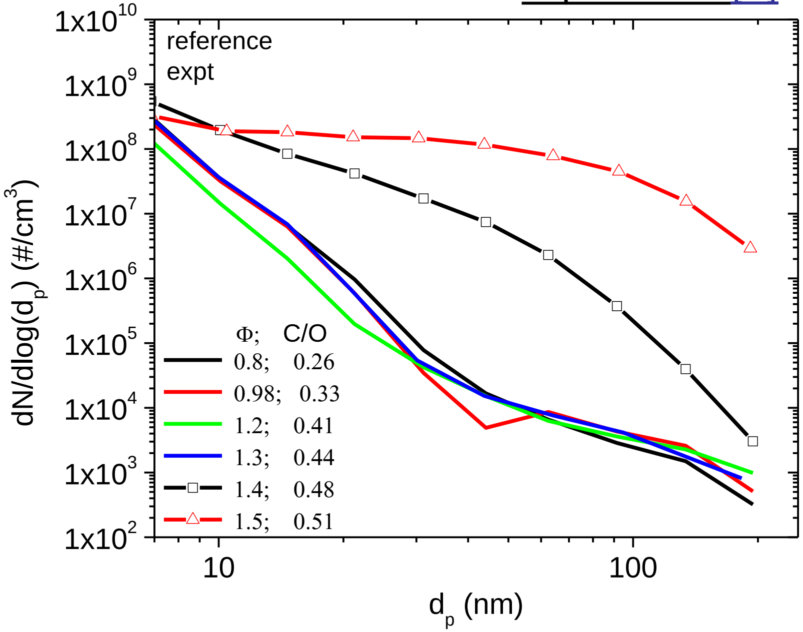
Jiao, 2014

80^0 ATDC ϕ =1.5

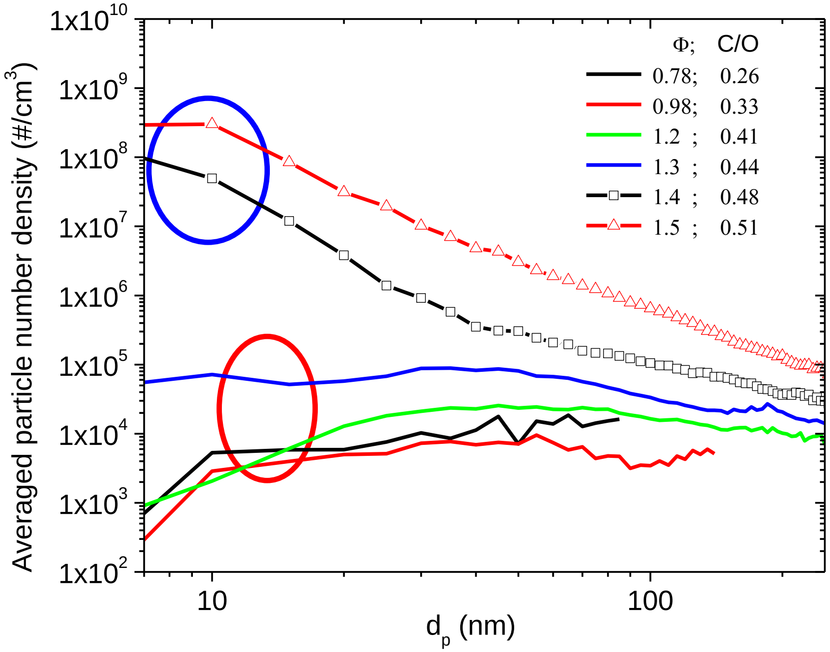


Particulate size distributions

Experiment [1]



Simulation



Nearly identical PSDs until about φ =1.3, nd sharply declines with increase of dp.

When φ >1.3, nd consistently increases with increasing φ , and decreases gradually with increasing dp.

For φ <1.4, shape of PSDs is very flat and broad, which is different from experiment, but looks like PSDs for A/F of 14.6 for engine loads lower than 4 bar in Ref. [2].

For φ =1.4 and 1.5 , magnitude of nd of small particles are well represented, nd decreases with increasing dp.

[1] Hageman, 2013. [2] Maricq, 1999

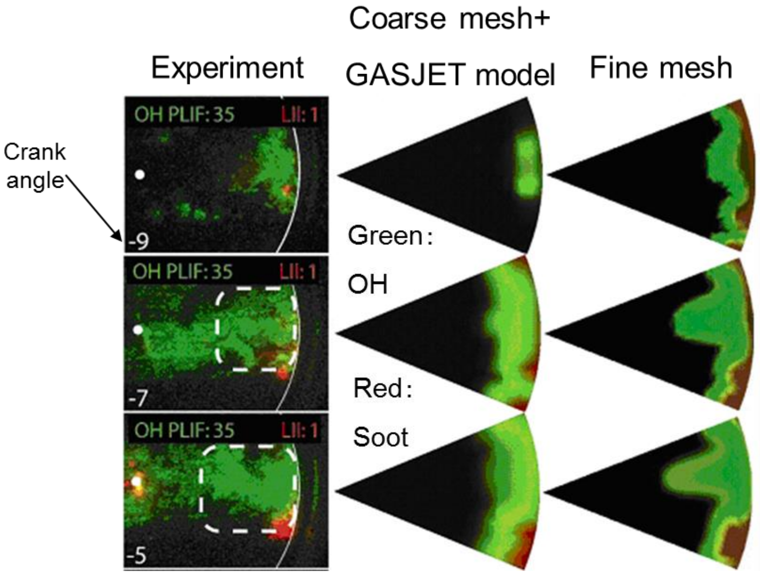
Vishwanathan, 2010

Soot in stratified charge engines

SANDIA optical engine – HTC/LTC

Engine	Parameter
Bore x stroke (cm)	13.97 x 15.24
Speed (rpm)	1200
Compression ratio (CR)	11.2:1
Swirl ratio	0.5
Number of nozzle holes	8
Orifice diameter (mm)	0.196
Included angle	152°
Fuel	Diesel #2
Sector angle	45

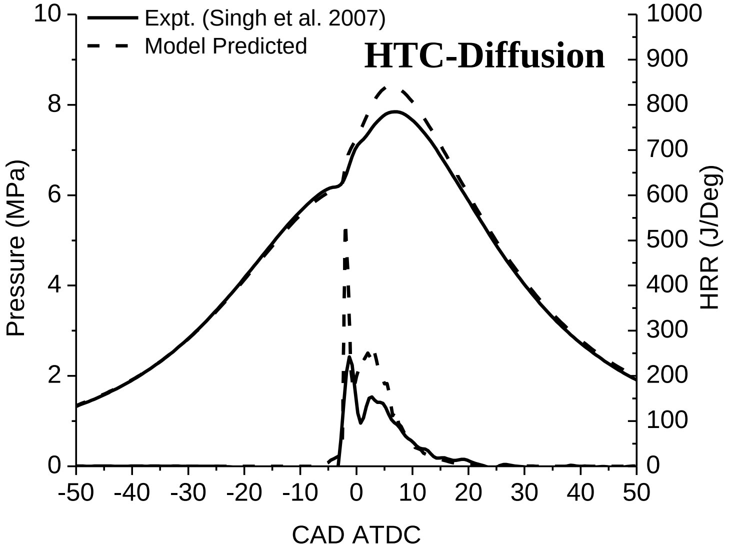
	HTC-diff./ premixed	LTC Early/late
Amb. O_2 %	21	12.7
SOI	-7/-5	-22/0
P_{in} (bar)	2.33/1.92	2.14/2.02
T_{in} (C)	111/47	90/70
Fuel (mg)	61	56
P_{inj} (bar)	1200	1600

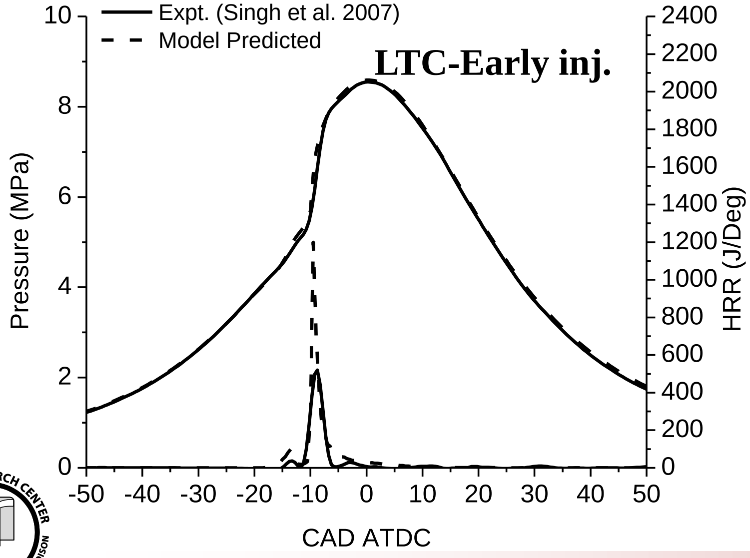


Expt. Data: Singh, 2007

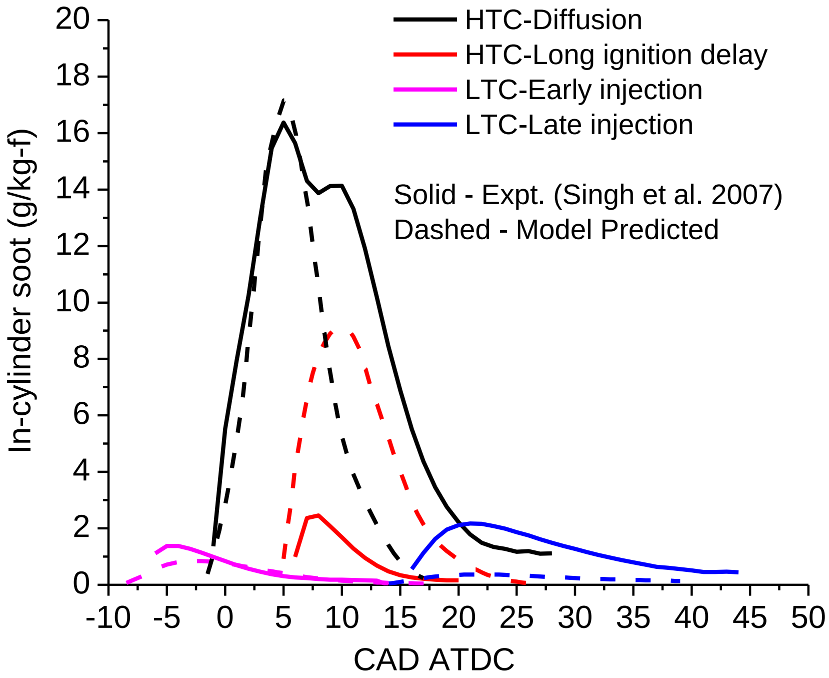
Vishwanathan, 2010

SNL optical engine – HTC/LTC





In-cylinder soot formation/oxidation
Difference in HTC and LTC soot amounts well captured

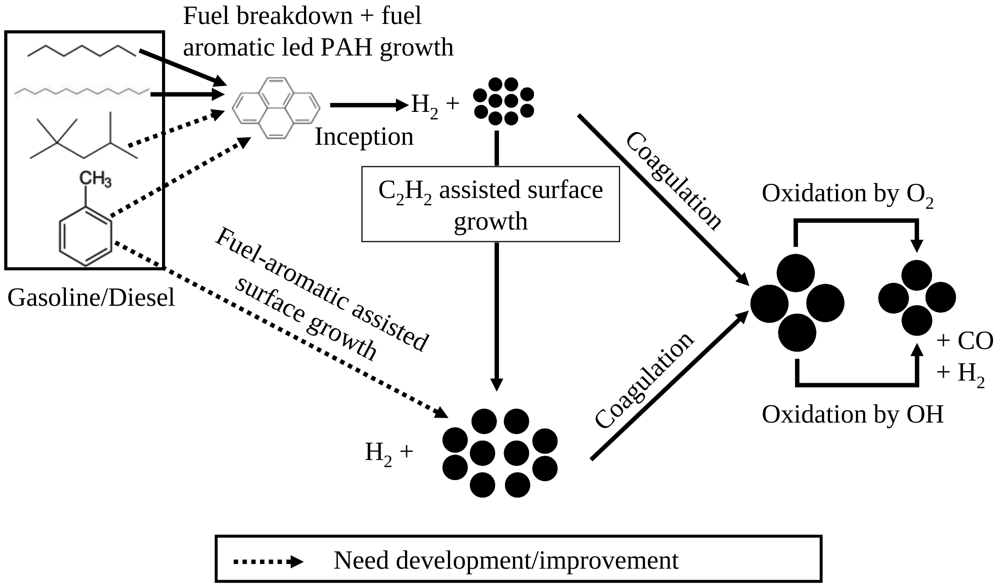


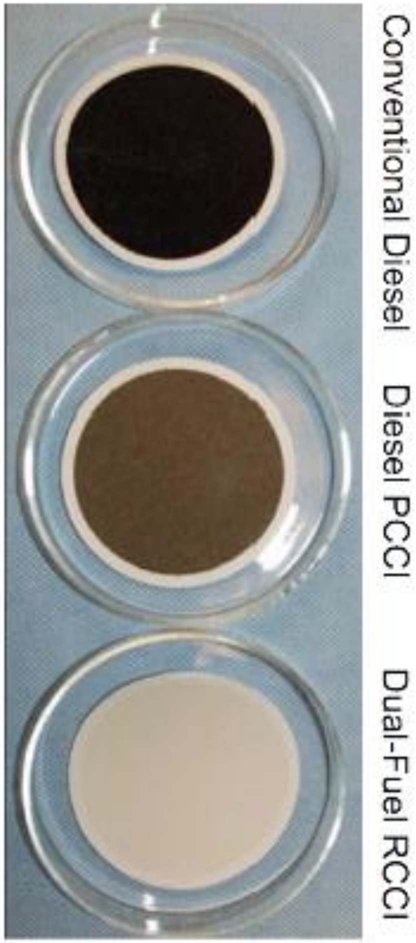
Diffusion to premixed combustion, soot ↓
HTC to LTC, soot ↓

Expt. Data: Singh, 2007

Summary and current directions

Integration of soot model with multi-component vaporization and chemistry models





Extension to GDI and H/P/RCCI

Organic fraction modeling:
OF correlates with premixedness

Soot diameter comparisons with TEM measurements obtained from various combustion modes