Computational Fluid Dynamics Modeling of Diesel Engine Combustion and Emissions

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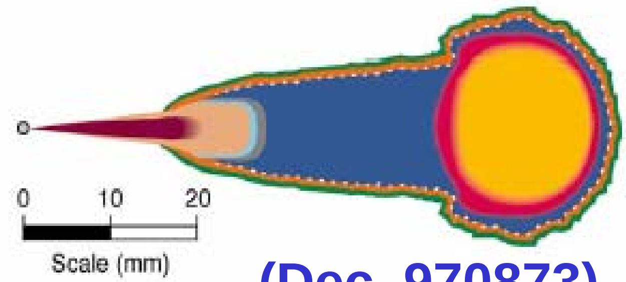
http://www.erc.wisc.edu/

Acknowledgments:
DOE/Sandia Labs; Caterpillar, Inc.; GM

Overview

- Introduction
  - Stringent future emission standards
  - Extensive experimental and theoretical studies of diesel spray combustion mechanisms in progress
    - Dec et al.; Pickett and Siebers; Musculus et a
    - Peters et al; Kong et al.; Golovitchev et al.
  - Detailed diesel flame structure shown to have important effects on emissions



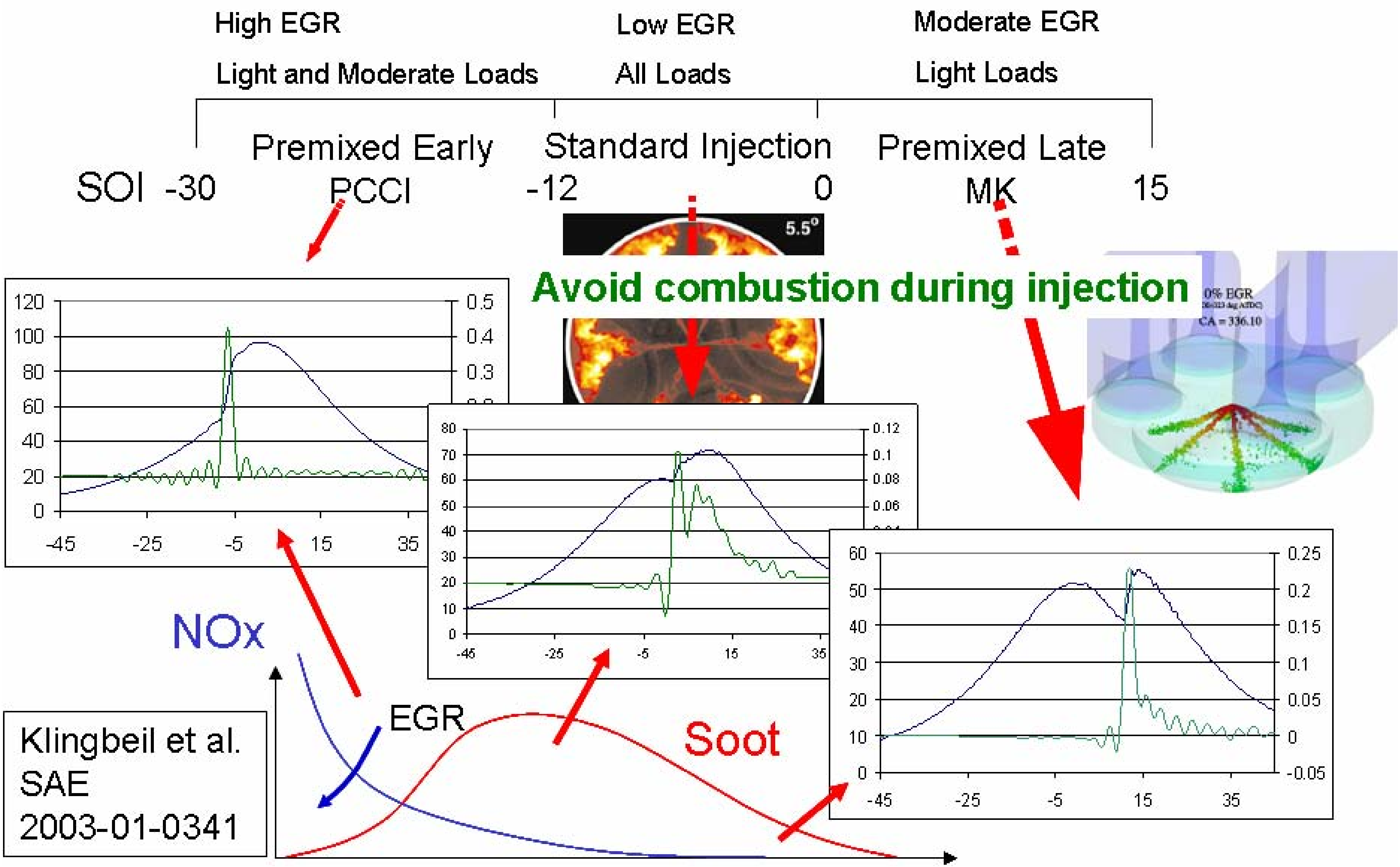
(Dec, 970873)

  - Low temperature combustion—partial-HCCI, PCCI concepts
  - Comprehensive reaction chemistry is needed for LTC modeling
- Objectives

— develop validated numerical models to study low- temperature (emission) diesel engine combustion (LTC)

— apply models to optimize LTC engine performance

Low temperature diesel combustion



1. Sandia spray experiments – model validation

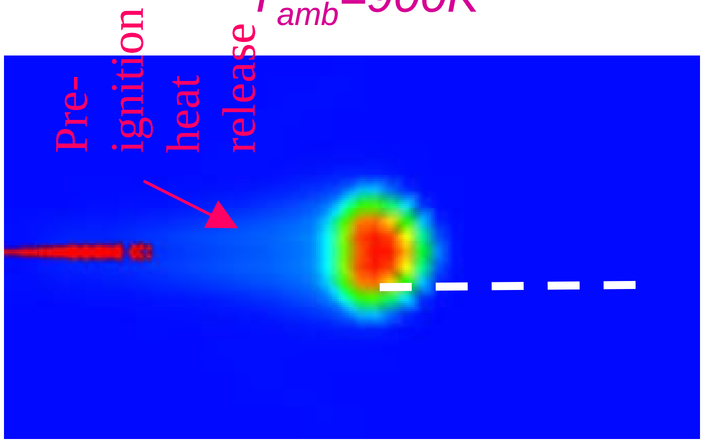
- **Non-sooting, low flame temperature experiments**
  - **Pickett and Siebers (SAE 2004-01-1399; *Comb. Flame*, 2004)**
  - **Sooting tendency of diesel spray at different operating conditions**

Experimental baseline conditions

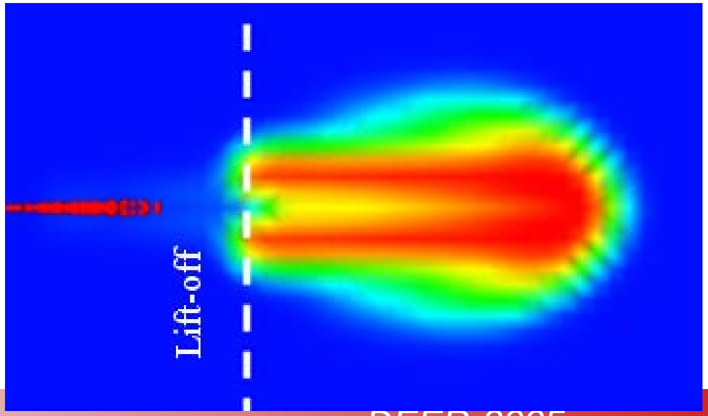
Fuel	D2
Injection system	Common-rail
Injection profile	Top-hat
Injector orifice	50, <u>100</u>, 180 µm
Orifice pressure drop	138 MPa
Discharge Coefficient	0.80
Fuel temperature	436 K
Ambient temperature	850, <u>900</u>, 1000 K
Ambient density	14.8 kg/m^3
O2 concentration	21%

Predicted T contours - T_{amb}=900K

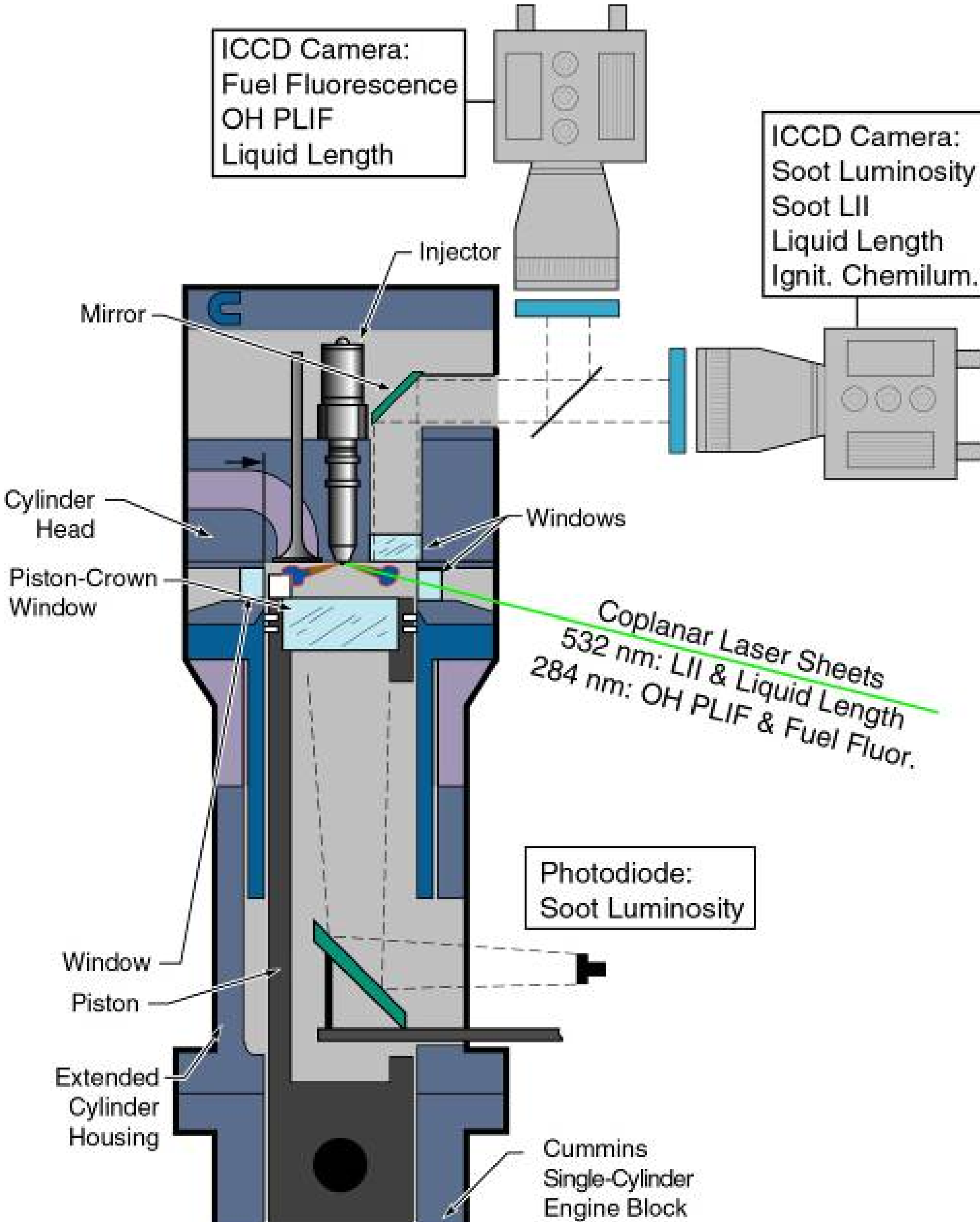
1.4 ms ASI



2.7 ms ASI



2. Sandia optical engine – in-cylinder validation



Sandia Cummins N14 Heavy-duty diesel engine

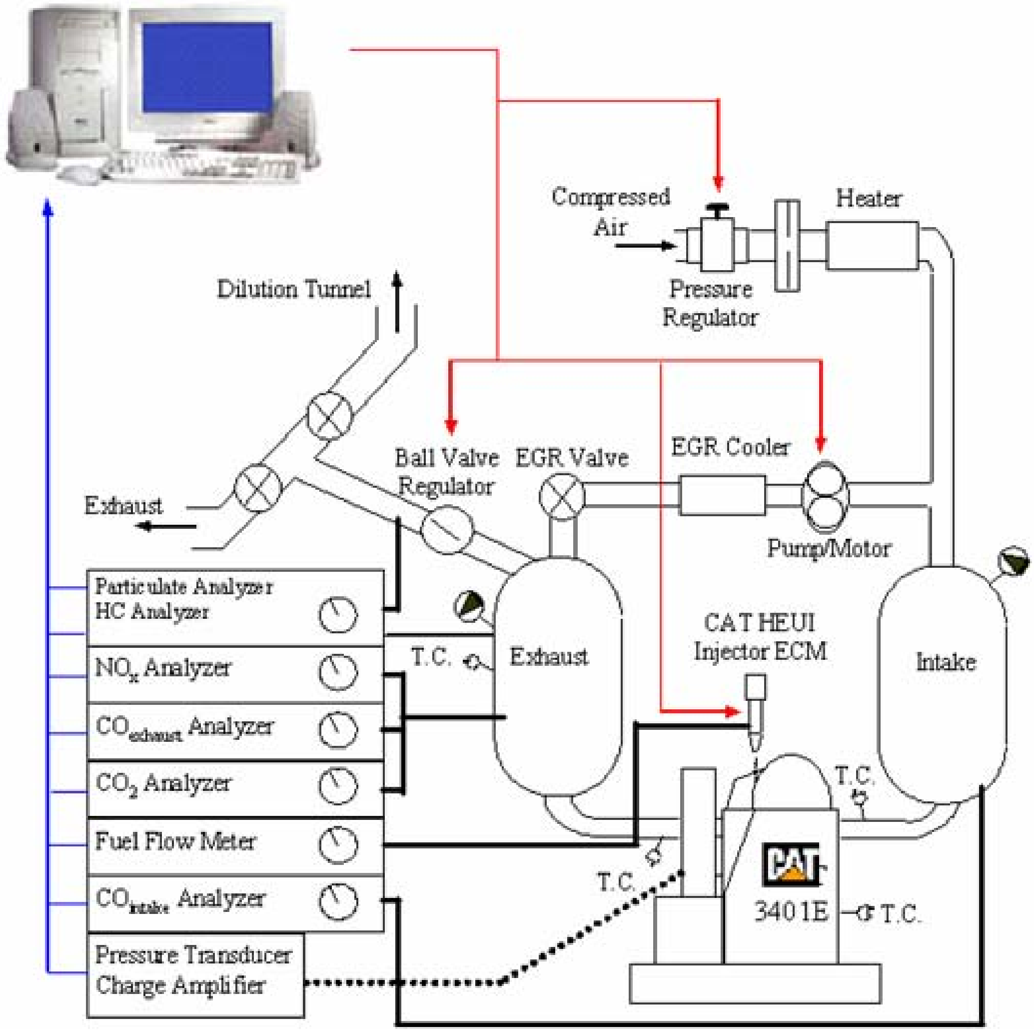
Singh, Musculus – SAE 05FFL-105

Diagnostics:

3-color soot thermometry and high speed imaging of soot luminosity
Liquid fuel penetration (Mie scattering)
OH planar laser induced fluorescence (PLIF)
Ignition chemiluminescence
Soot laser induced incandescence (LII)
Fuel fluorescence vapor fuel image
Exhaust NOx measurement

3. ERC diesel engine NOx and Soot emissions

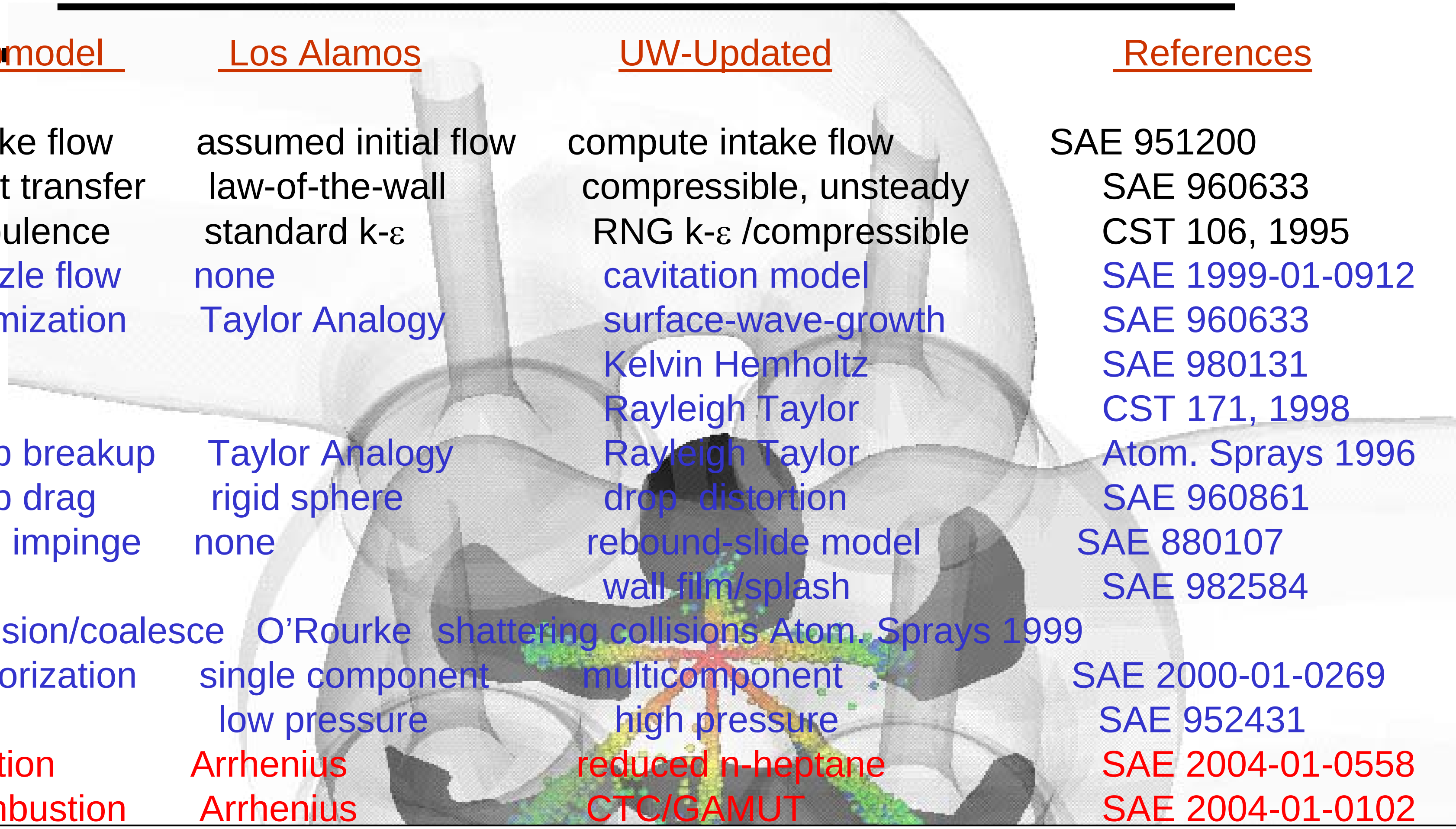
- Caterpillar 3401 SCOTE – Class 8 truck



Engine	Caterpillar 3401 SCOTE (Single Cylinder Oil Test Engine) - single cylinder - direct injection - 4 valve
Bore x Stroke	137.2 mm x 165.1 mm
Compression Ratio	16.1 : 1
Displacement	2.44 liters
Combustion Chamber	Quiescent
Piston	Mexican Hat with SharpEdge Crater
HUEI injector	3 pulse injections

Operated near PCCI for low emissions
Various SOI (-20 to +5 ATDC)
Various EGR (8 to 40%)

UW-ERC multidimensional modeling – KIVA3V



Submodel	Los Alamos	UW-Updated	References
intake flow	assumed initial flow	compute intake flow	SAE 951200
heat transfer	law-of-the-wall	compressible, unsteady	SAE 960633
turbulence	standard k-ε	RNG k-ε /compressible	CST 106, 1995
nozzle flow	none	cavitation model	SAE 1999-01-0912
atomization	Taylor Analogy	surface-wave-growth	SAE 960633
		Kelvin Hemholtz	SAE 980131
		Rayleigh Taylor	CST 171, 1998
drop breakup	Taylor Analogy	Rayleigh Taylor	Atom. Sprays 1996
drop drag	rigid sphere	drop distortion	SAE 960861
wall impinge	none	rebound-slide model	SAE 880107
		wall film/splash	SAE 982584
collision/coalesce	O'Rourke	shattering collisions	Atom. Sprays 1999
vaporization	single component	multicomponent	SAE 2000-01-0269
	low pressure	high pressure	SAE 952431
ignition	Arrhenius	reduced n-heptane	SAE 2004-01-0558
combustion	Arrhenius	CTC/GAMUT	SAE 2004-01-0102

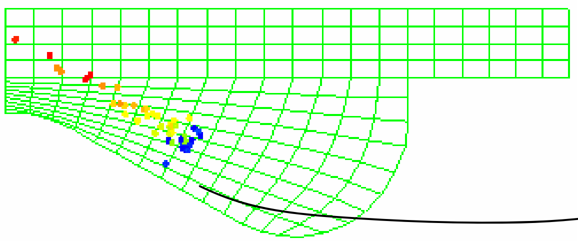
ignition	Arrhenius	reduced n-heptane	SAE 2004-01-0558
combustion	Arrhenius	CTC/GAMUT	SAE 2004-01-0102
		reduced kinetics	SAE 2003-01-1087
NOx	Zeldo'vich	Extended Zeldo'vich	SAE 940523
soot	none	Hiroyasu & Surovkin	SAE 960633
		Nagle Strickland oxidation	SAE 980549

KIVA-ERC + CHEMKIN for LTC modeling

- CFD code coupled with detailed chemistry

Reaction Mechanism
Thermodynamic Data

CFD Code



Interface:

$\rho_k(\mathrm{x}), \Delta e(\mathrm{x})$

CHEMKIN Utilities

$$\begin{cases} \frac{dY_k}{dt} = v\dot{\omega}_k W_k \\ c_v \frac{dT}{dt} + v\sum_{k=1}^{K} e_k \dot{\omega}_k W_k = 0 \end{cases}$$

  - Interface Utility—exchange cell information between KIVA and CHEMKIN
- Fuel oxidation chemistry
  - Skeletal n-heptane mech (30 species, 65 reactions)
  - SENKIN, XSENKPLOT, GA (Patel et al., SAE 2004-01-0558)
  - Parallel computing

NOx and Soot emission models

Kong et al. ASME Spring Technical Conference, Paper ICES2005-1009

- NO/NO2 formation mechanism
  - Reduced from GRI NO mechanism
  - extra 4 species (N, NO, NO2, N2O) and 9 reactions
- Soot model—phenomenological
  - Competing formation and oxidation rates
  - Hiroyasu-type formation rate and NSC oxidation reactions
  - Acetylene (C_2H_2) is used as the "soot formation species"

$$A_f M_{fv} P^{0.5} \exp(-E/RT)$$ ← **Hiroyasu**

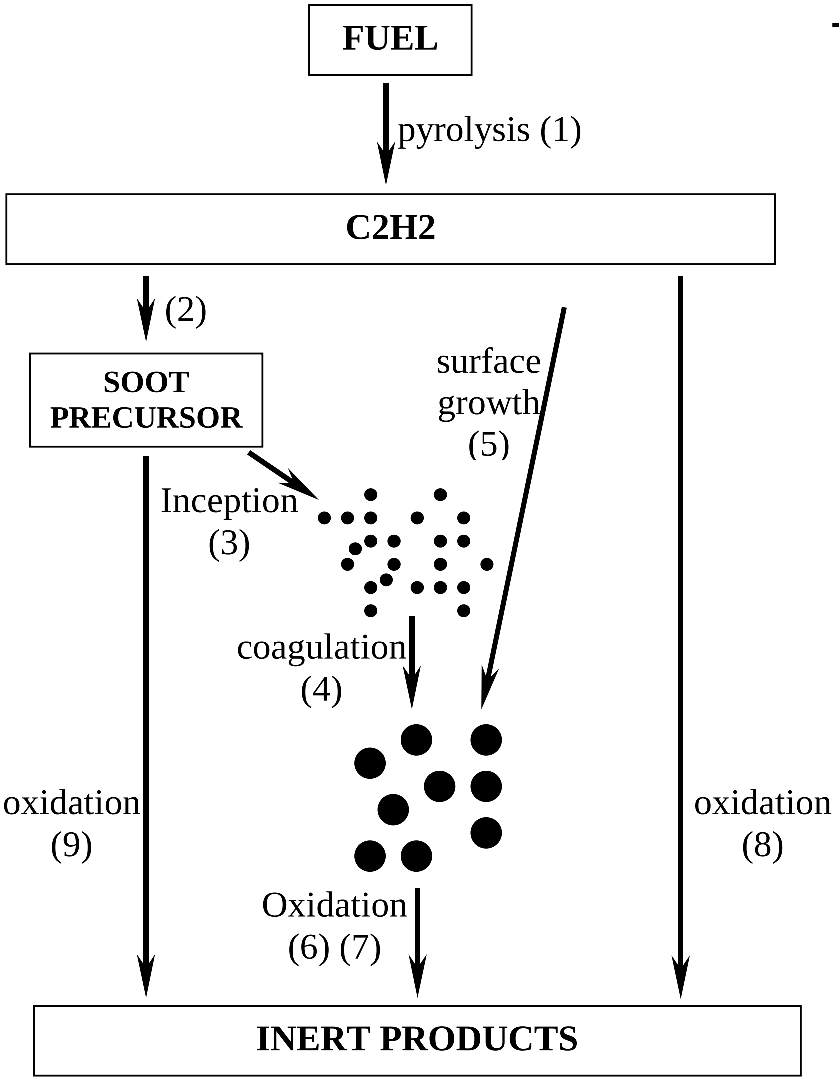
$$dM_{net} = dM_{form} - dM_{oxid}$$

NSC → $$\frac{6Mw_c}{\rho_s D_s} M_s R_{Total}$$

$$\begin{cases} R_{Total} = \left\{ \left(\frac{K_A P_{O2}}{1 + K_Z P_{O2}} \right) x + K_B P_{O2} (1 - x) \right\} Mw_c \\ x = \frac{P_{O2}}{P_{O2} + (K_T / K_B)} \end{cases}$$

(fraction of reactive 'A' sites)

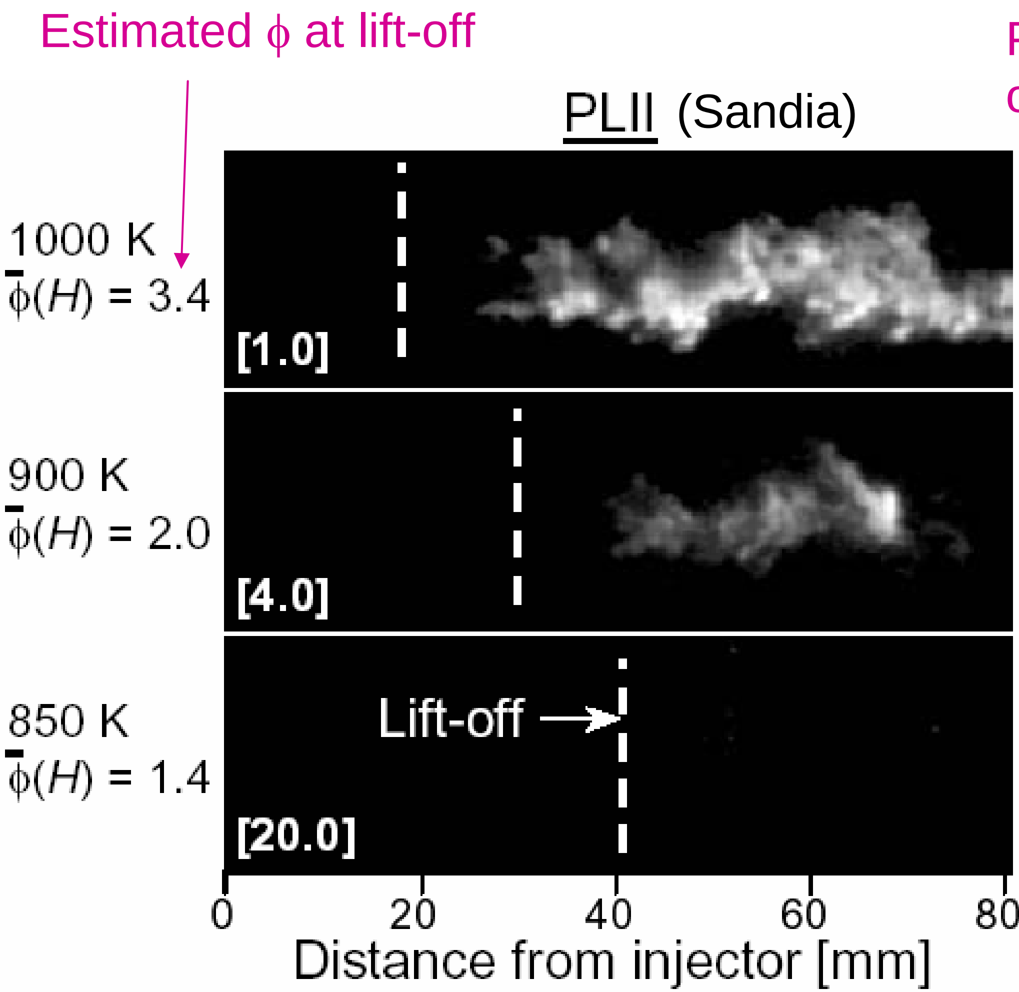
Multi-step phenomenological soot model



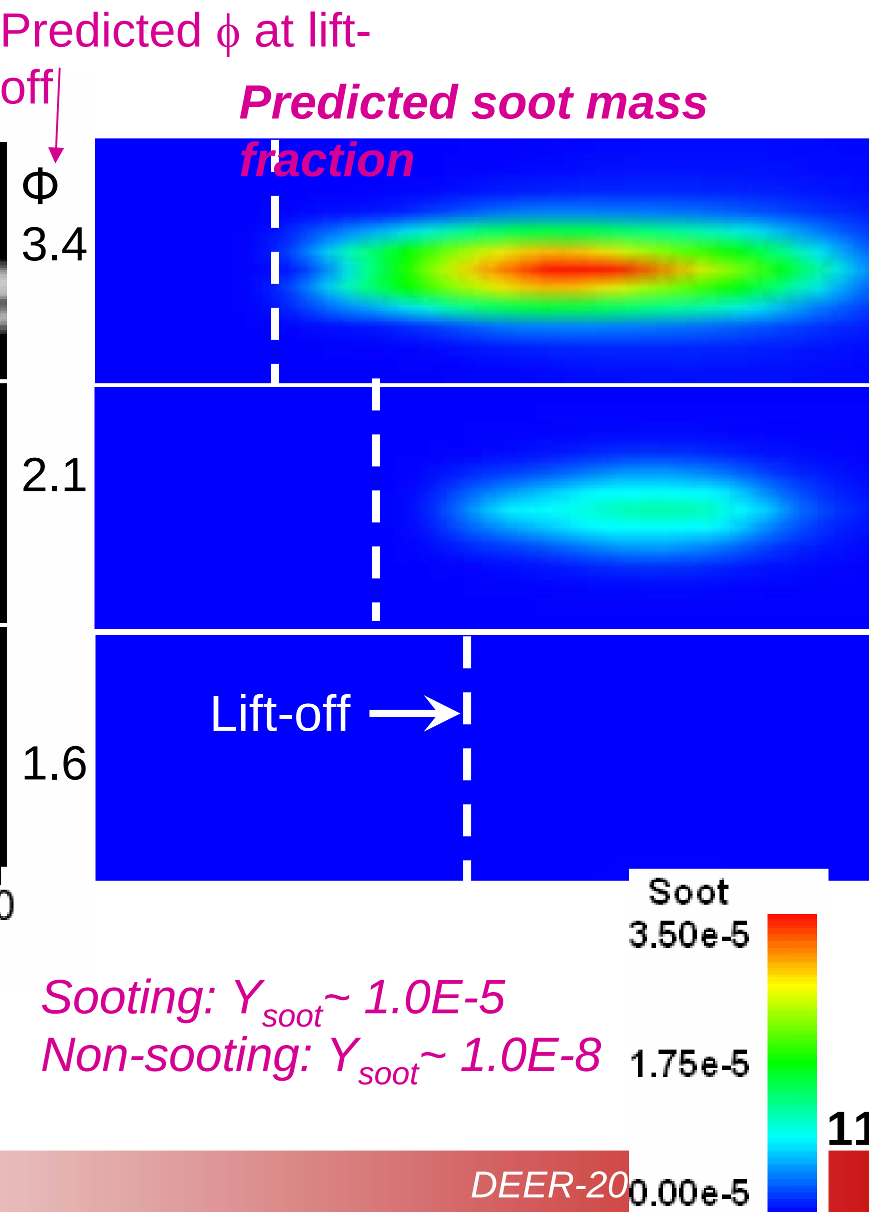
Tao et al. SAE Paper 2005-01-0121

1. $Fuel \rightarrow C_2H_2$
2. $C_2H_2 \rightarrow R$
3. $R \rightarrow C_{soot}$
4. $xC_{soot} \rightarrow C_{soot}$
5. $C_{soot} + C_2H_2 \rightarrow C_{soot+2} + H_2$
6. $C_{soot} + O_2 \rightarrow C_{soot-2} + 2CO$
7. $C_{soot} + OH \rightarrow CO + \frac{1}{2}H_2$
8. $C_2H_2 + O_2 \rightarrow 2CO + H_2$
9. $R + O_2 \rightarrow product$

Spatial soot contours



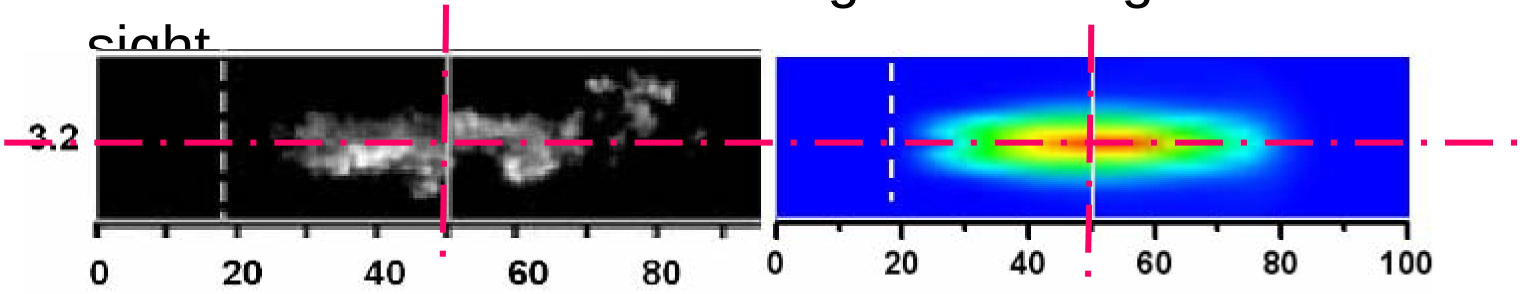
varying Tamb @ 3.2 ms



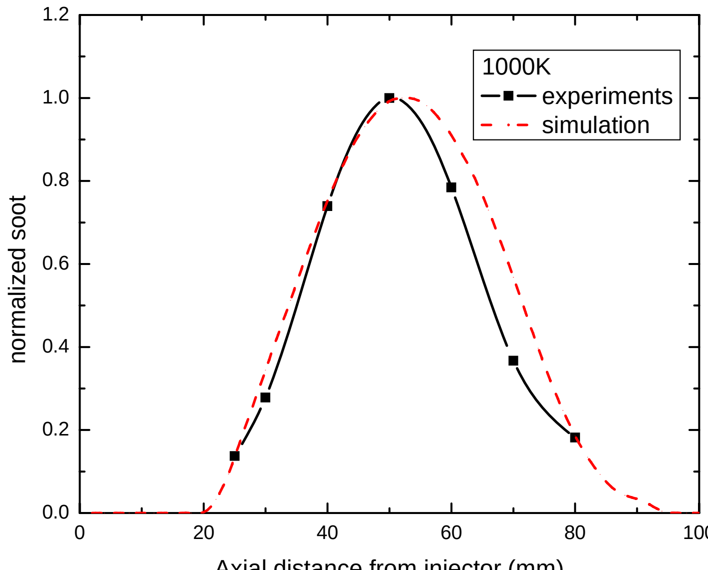
Sooting: Y_{soot}~ 1.0E-5
Non-sooting: Y_{soot}~ 1.0E-8

Axial and radial soot distributions

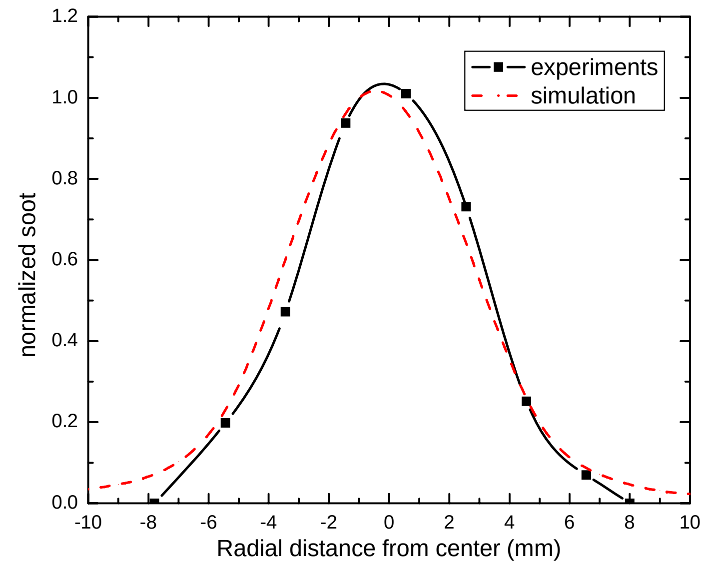
- Qualitative comparisons—normalized data @ 3.2 ms
  - Experiments—KL factor, derived from laser-extinction expt
  - Simulations—soot mass integrated along the same line of sight



Axial distributions along spray axis

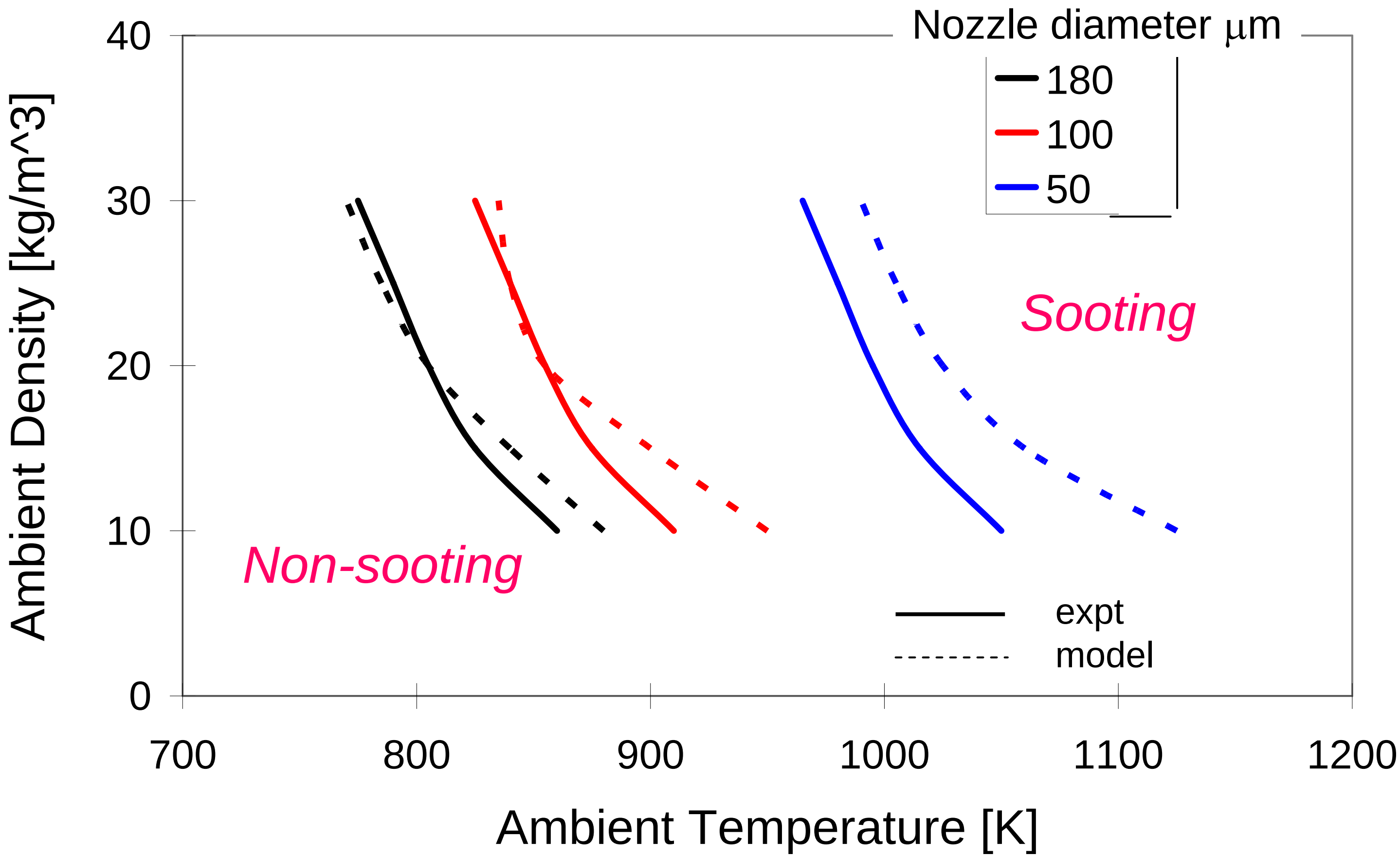


Radial distributions along 50 mm line

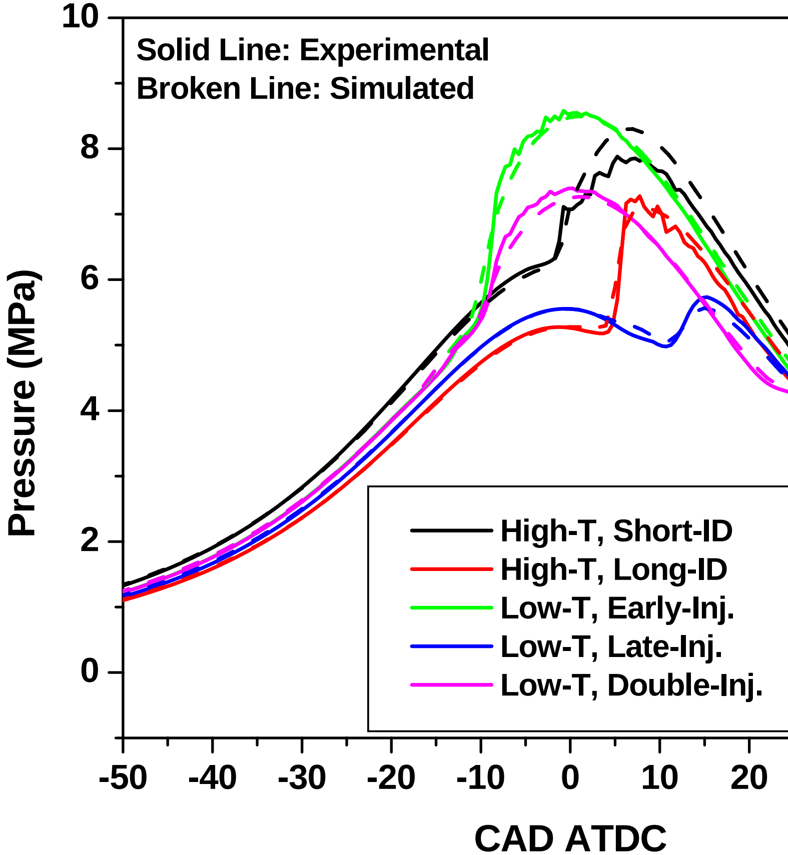


Sooting regimes using multi-step soot model

- Sandia spray sooting exp't for P_{inj}=138 MPa
- Sooting tendency of diesel spray is well predicted



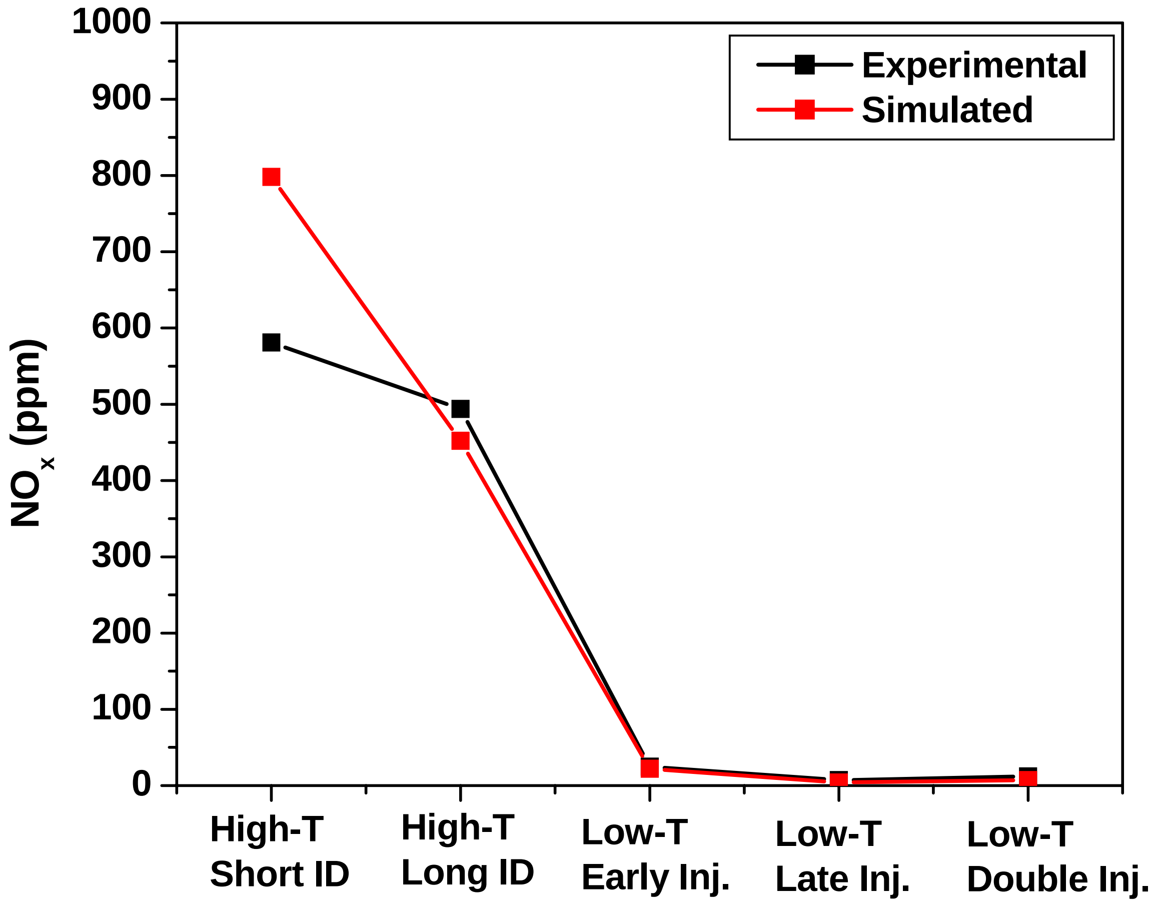
Sandia/Cummins N14 – multi-mode combustion

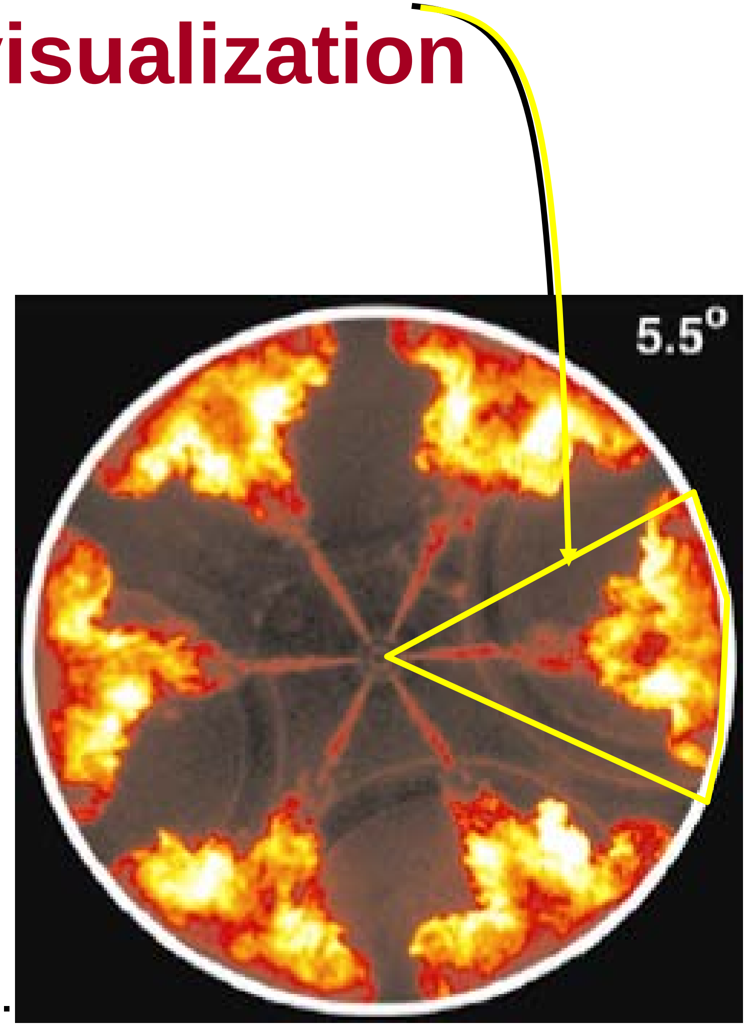


	High-T Short-ID - Diffusion combustion	High-T, Long-ID - Premixed combustion	Low-T, Early-Inj. (Lean Premixed)	Low-T, Late-Inj. (MK)	Low-T, Double-Inj. (UNIBUS)
Speed (RPM)	1200	1200	1200	1200	1200
IMEP (bar)	4	4	4	4	4
Injection Pressure (bar)	1200	1200	1600	1600	1600
Intake Temp (°C)	111	47	90	70	90
Intake Pressure (kPa)	233	192	214	202	214
TDC Motored Temp. (K)	900	750	867	819	867
TDC Mot. Density (kg/m3)	24	24	24	24	24
SOI (°ATDC)	-7	-5	-22	0	– 22, + 15
Injection Quantity (mg)	61	61	56	56	31, 33
DOI (CAD)	10	10	7	7	4, 4
O_2 Conc. (Vol %)	21	21	12.6	12.6	12.6

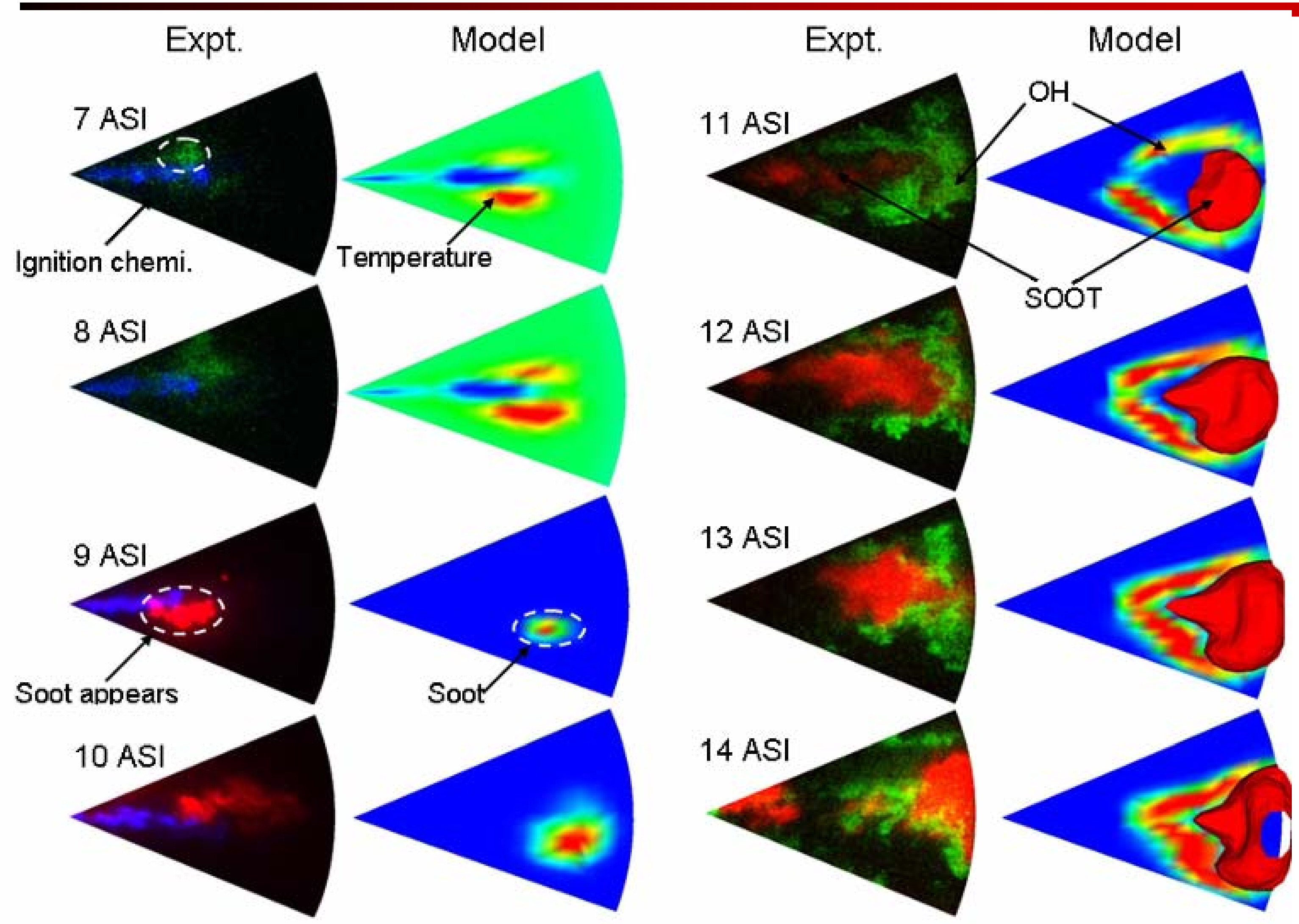
MK: Kimura SAE 2001-01-0200
UNIBUS: Hasegawa, Yanagihara SAE 2003-01-0745

Sandia/Cummins N14 – NOx and combustion visualization



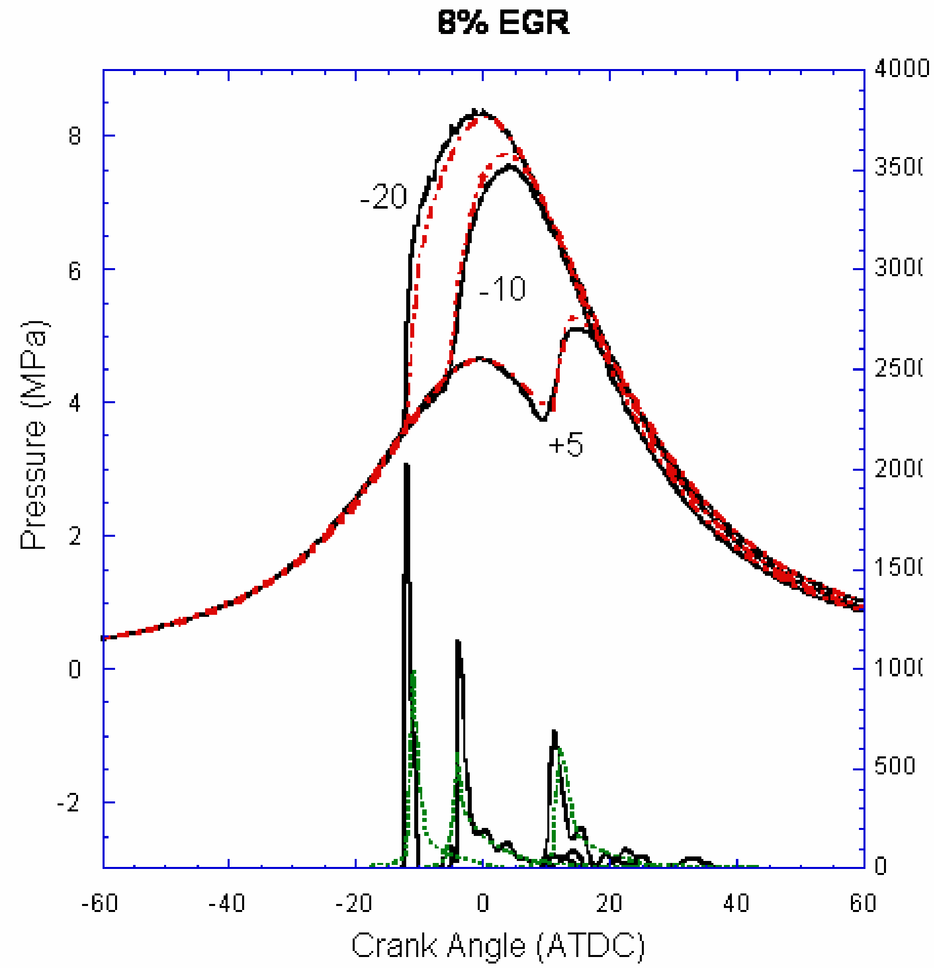


In-cylinder comparisons - premixed combustion

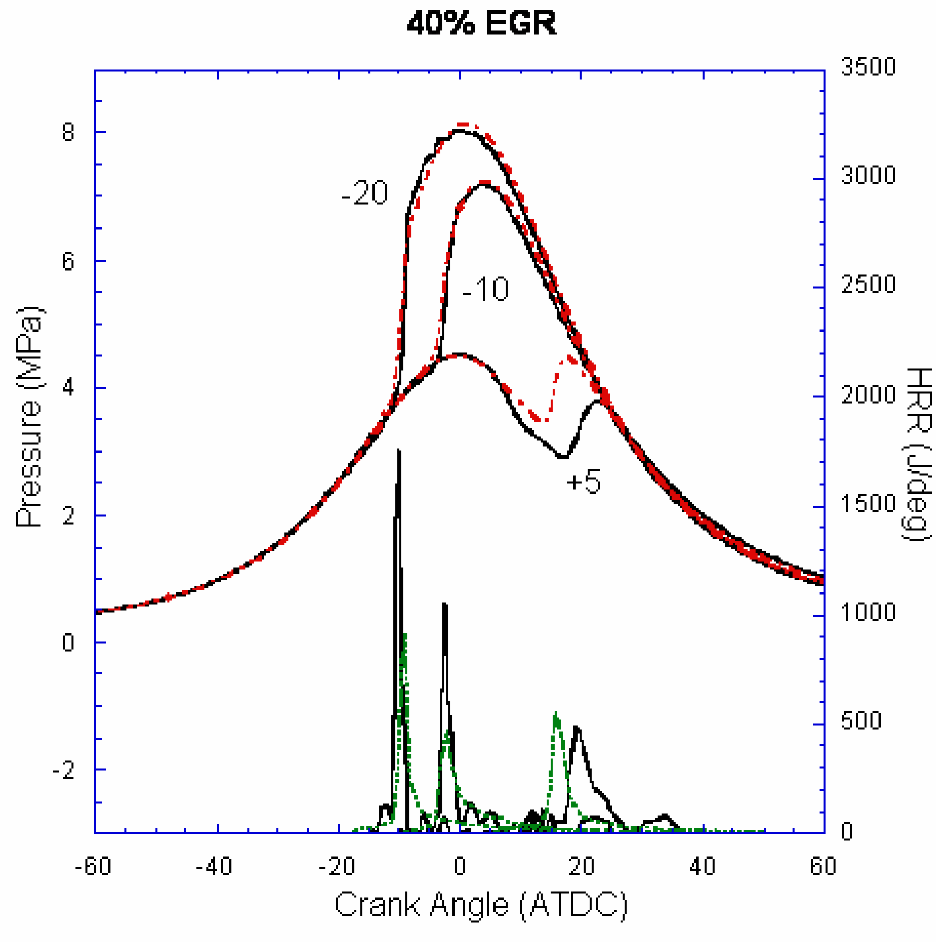


Camera gain 10x less than std. diesel

ERC Caterpillar engine combustion predictions



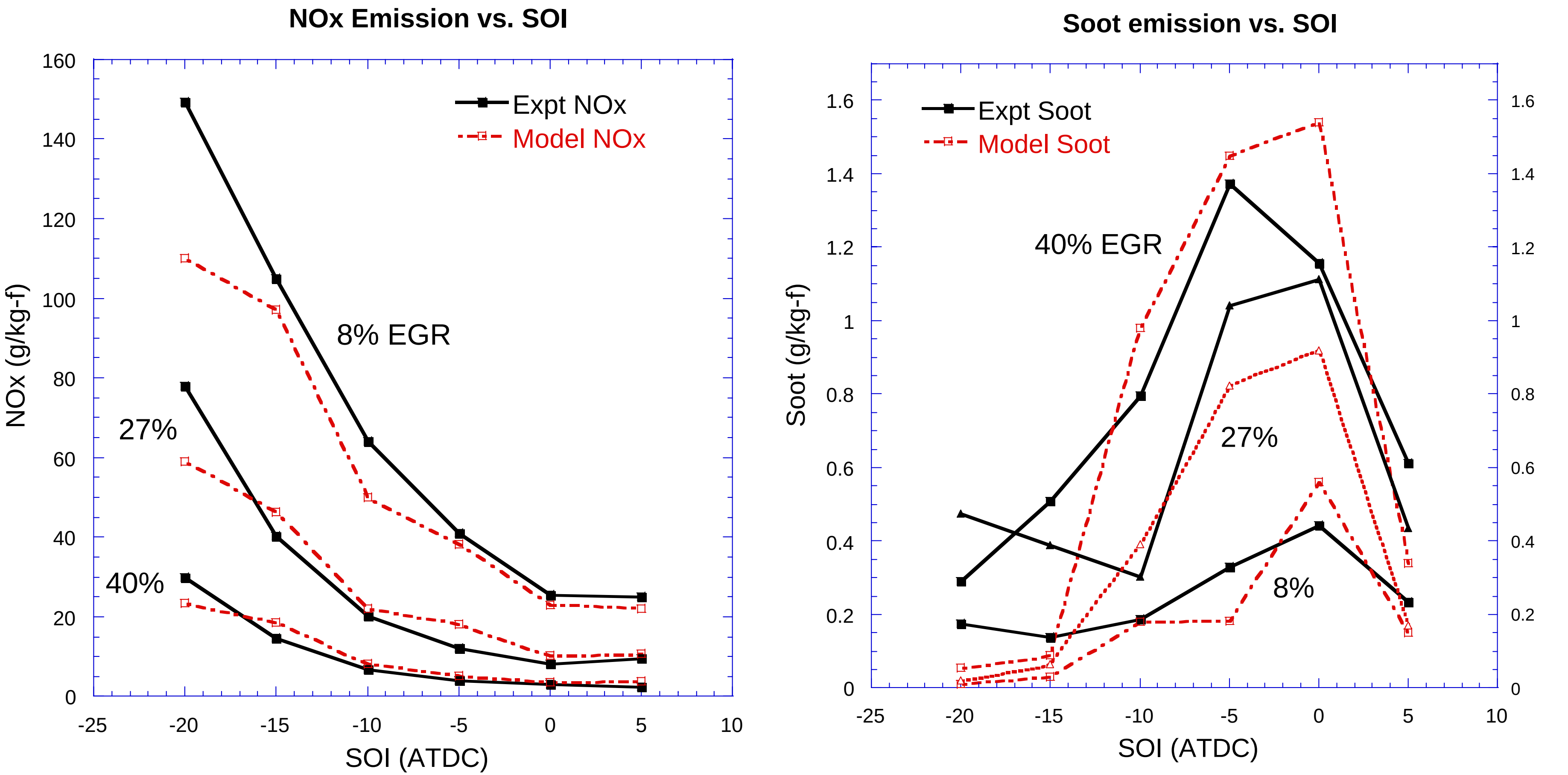
Highly premixed combustion characteristics



- 821 rpm, 25% load cooled EGR

ERC Caterpillar NOx & Soot emission predictions

– Low soot emissions at low ambient temperature, similar to Sandia spray vessel results



Model application - Diesel LTC challenges

Tradeoff

Vaporization too slow | Ignition too fast

Charge preparation

Prevent wall films - unburned fuel

Enablers: Advanced injection concepts

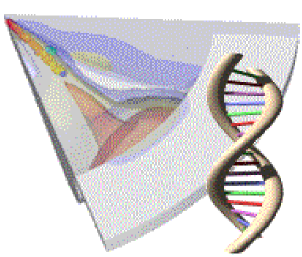
- Ultra-high injection pressure
- Optimized piston/spray geometry (NADI)
- Variable Geometry Sprays
- Short multiple pulse injection
- Impinging sprays

In-cylinder thermodynamics

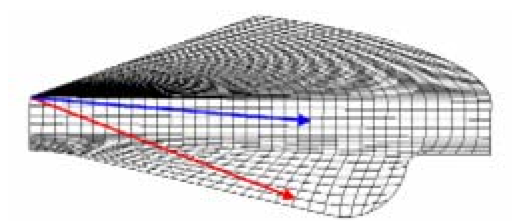
Compression press/temp - phasing

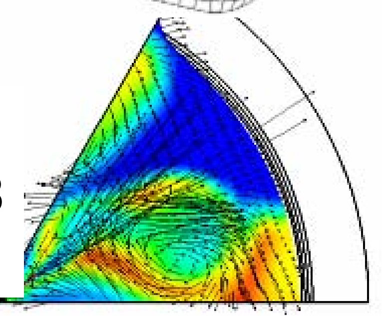
Enablers: Advanced engine controls

- Variable Valve Timing
- Two-stage turbo-charging
- EGR
- Compression ratio control
- Fuel CN reduction



Genetic Algorithm optimization
Engine design



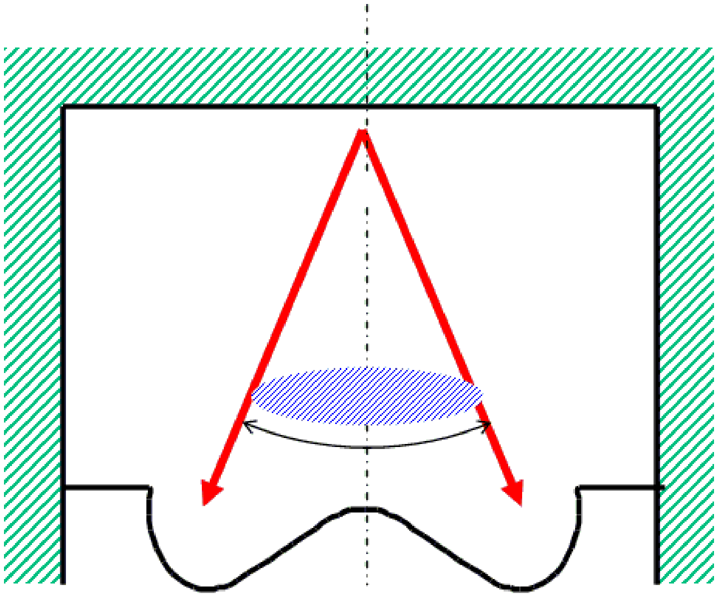


Bergin - Spin-spray Combustion: SAE 2005-01-0916

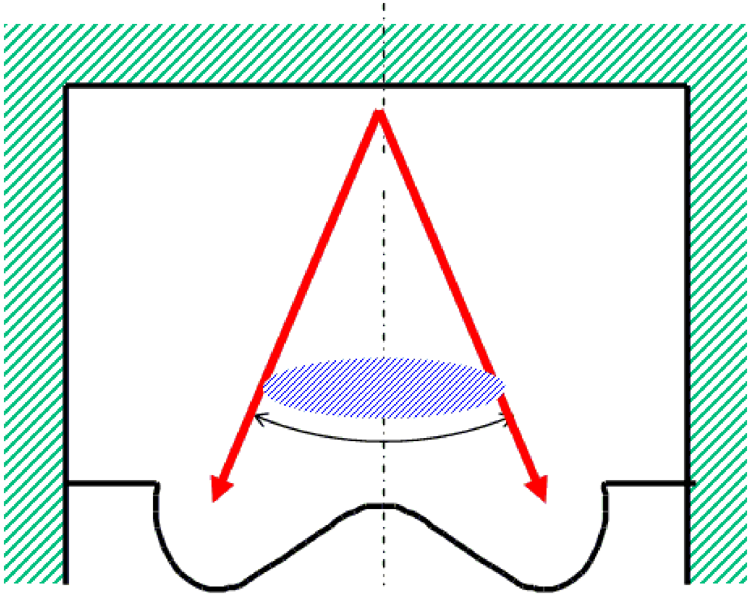
Wickman - Optimized Piston Geometry: SAE 2003-01-0348

Ra, Sun – optimized VGS: SAE 2005-01-0148, ILASS-05

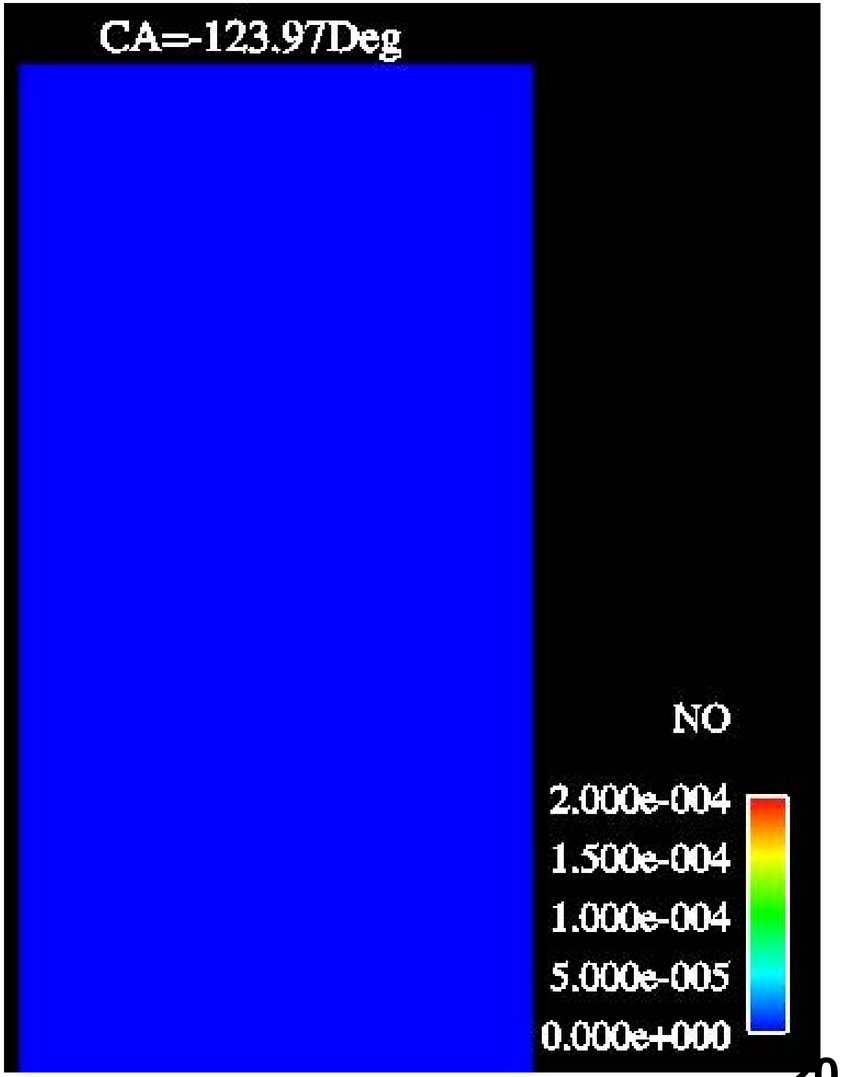
Variable geometry sprays



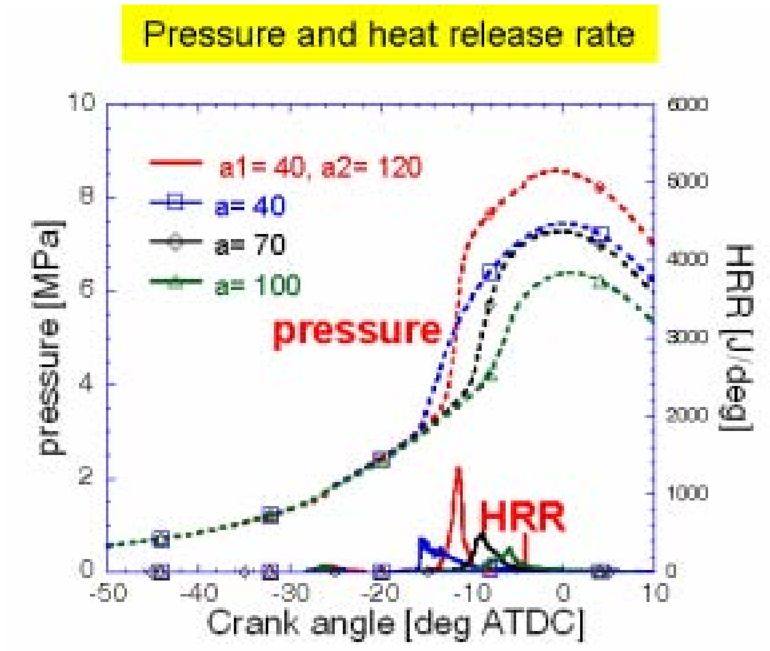
Two-
Pulse
Sprays

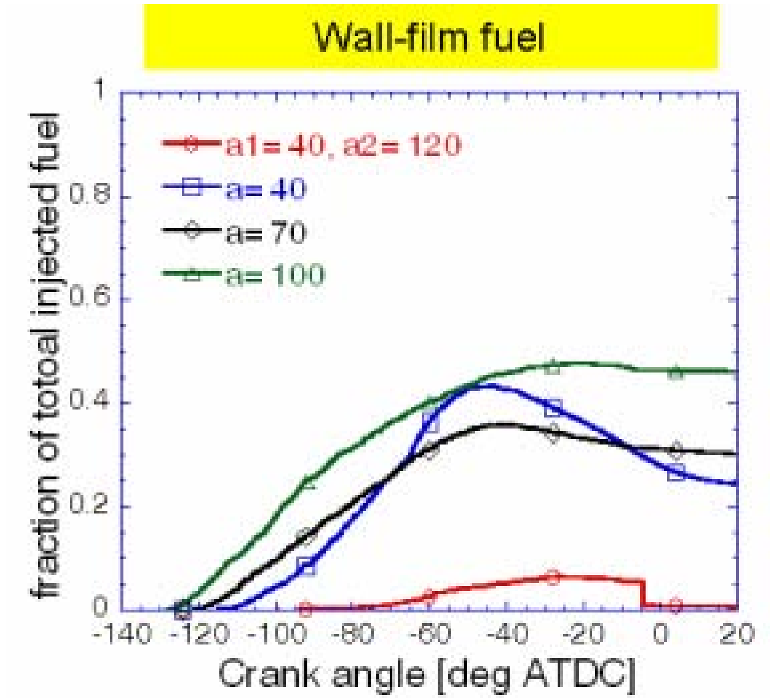


GA optimized low pressure injection



Variable geometry sprays





SOI= -143 deg ATDC

Comparison between VGS and three fixed spray angle cases

SOI= -143 deg ATDC

VGS has potential to decrease wall impingement compared to single fixed angle sprays

Summary and Conclusions

- Future engines will employ advanced combustion concepts with sophisticated injection control strategies (e.g., multiple injection, VGS) and variable valve timing
- Available CFD combustion modeling captures emission trends and can be used for design of advanced engines
- Models useful to help explain emission trends – e.g.,
  - as ambient temperature is decreased, flame lift-off length is increased and soot emission is reduced due to better mixing
  - soot emission is decreased at retarded SOI as a result of better mixing and low-temperature combustion—less soot is formed
- Advanced injection concepts can significantly reduce spray wall impingement for improved charge preparation.
  Late intake valve closure useful for combustion phasing control in LTC regime.
- Optimization is needed for combustion chamber/spray matching.
- Further model improvements are in progress in the areas of:
  - more grid independent spray models
  - integration of detailed chemical kinetics models for realistic fuels
  - coupling detailed kinetics and turbulent flame propagation models (G-models)
  - assessment of the effects of turbulence on LTC combustion (LES models)