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 al.
    • Peters et al; Kong et al.; Golovitchev et al.
  – Detailed diesel flame structure shown to have important effects on emissions
  – 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

High EGR
Light and Moderate Loads

-30 SOI
Premixed Early
PCCI

Low EGR
All Loads

-12 Standard Injection
0

Moderate EGR
Light Loads

15 Premixed Late
MK

Avoid combustion during injection

NOx
EGR
Soot

Klingbeil et al.
SAE
2003-01-0341
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**

<table>
<thead>
<tr>
<th>Fuel</th>
<th>D2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection system</td>
<td>Common-rail</td>
</tr>
<tr>
<td>Injection profile</td>
<td>Top-hat</td>
</tr>
<tr>
<td>Injector orifice</td>
<td>50, 100, 180 μm</td>
</tr>
<tr>
<td>Orifice pressure drop</td>
<td>138 MPa</td>
</tr>
<tr>
<td>Discharge Coefficient</td>
<td>0.80</td>
</tr>
<tr>
<td>Fuel temperature</td>
<td>436 K</td>
</tr>
<tr>
<td>Ambient temperature</td>
<td>850, 900, 1000 K</td>
</tr>
<tr>
<td>Ambient density</td>
<td>14.8 kg/m³</td>
</tr>
<tr>
<td>O₂ concentration</td>
<td>21%</td>
</tr>
</tbody>
</table>

*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

<table>
<thead>
<tr>
<th>Engine</th>
<th>Caterpillar 3401 SCOTE (Single Cylinder Oil Test Engine)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>single cylinder</td>
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<tr>
<td></td>
<td>direct injection</td>
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<td></td>
<td>4 valve</td>
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</table>

<table>
<thead>
<tr>
<th>Bore x Stroke</th>
<th>137.2 mm x 165.1 mm</th>
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</thead>
<tbody>
<tr>
<td>Compression Ratio</td>
<td>16.1 : 1</td>
</tr>
<tr>
<td>Displacement</td>
<td>2.44 liters</td>
</tr>
<tr>
<td>Combustion Chamber</td>
<td>Quiescent</td>
</tr>
<tr>
<td>Piston</td>
<td>Mexican Hat with SharpEdge Crater</td>
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<tr>
<td>HUEI injector</td>
<td>3 pulse injections</td>
</tr>
</tbody>
</table>

Operated near PCCI for low emissions
Various SOI (-20 to +5 ATDC)
Various EGR (8 to 40%)
## UW-ERC multidimensional modeling – KIVA3V

<table>
<thead>
<tr>
<th>Submodel</th>
<th>Los Alamos</th>
<th>UW-Updated</th>
<th>References</th>
</tr>
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<tbody>
<tr>
<td>intake flow</td>
<td>assumed initial flow</td>
<td>compute intake flow</td>
<td>SAE 951200</td>
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<td>heat transfer</td>
<td>law-of-the-wall</td>
<td>compressible, unsteady</td>
<td>SAE 960633</td>
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<tr>
<td>turbulence</td>
<td>standard k-ε</td>
<td>RNG k-ε /compressible cavitation model</td>
<td>CST 106, 1995</td>
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<td>nozzle flow</td>
<td>none</td>
<td>surface-wave-growth</td>
<td>SAE 1999-01-0912</td>
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<td>atomization</td>
<td>Taylor Analogy</td>
<td>Kelvin Hemholtz</td>
<td>SAE 960633</td>
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<td>Rayleigh Taylor</td>
<td>SAE 980131</td>
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<td>drop – distortion</td>
<td>CST 171, 1998</td>
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<td>rebound-slide model</td>
<td>Atom. Sprays 1996</td>
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<td></td>
<td></td>
<td>wall film/splash</td>
<td>SAE 960861</td>
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<td>collision/coalescence</td>
<td>SAE 880107</td>
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<td></td>
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<td>vaporization</td>
<td>SAE 982584</td>
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<tr>
<td></td>
<td></td>
<td>ignition</td>
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<tr>
<td></td>
<td></td>
<td>combustion</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>ignition</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>NOx</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>soot</td>
<td></td>
</tr>
</tbody>
</table>

### References:

- SAE 940523
- SAE 960549
- SAE 960633
- SAE 980549
KIVA-ERC + CHEMKIN for LTC modeling

- CFD code coupled with detailed chemistry

- 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

\[ \frac{dY_k}{dt} = v \omega_k W_k \]
\[ c_v \frac{dT}{dt} + v \sum_{k=1}^{K} e_k \dot{\omega}_k W_k = 0 \]
NOx and Soot emission models


- **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 (C₂H₂) is used as the "soot formation species"

\[
dM_{net} = dM_{form} - dM_{oxid}
\]

Hiroyasu

\[
\frac{6M_{Wc}}{\rho_s D_s} M_s R_{Total} = \frac{P_{O2}}{P_{O2} \left( K_T / K_B \right)}
\]

\[
R_{Total} = \left\{ \frac{K_A P_{O2}}{1 + K_Z P_{O2}} \right\} x + K_B P_{O2} \left( 1 - x \right) M_{Wc}
\]

(fraction of reactive ‘A’ sites)
Multi-step phenomenological soot model

Tao et al. SAE Paper 2005-01-0121

1. $\text{Fuel} \rightarrow \text{C}_2\text{H}_2$
2. $\text{C}_2\text{H}_2 \rightarrow R$
3. $R \rightarrow \text{C}_{\text{soot}}$
4. $x\text{C}_{\text{soot}} \rightarrow \text{C}_{\text{soot}}$
5. $\text{C}_{\text{soot}} + \text{C}_2\text{H}_2 \rightarrow \text{C}_{\text{soot}+2} + \text{H}_2$
6. $\text{C}_{\text{soot}} + \text{O}_2 \rightarrow \text{C}_{\text{soot}-2} + 2\text{CO}$
7. $\text{C}_{\text{soot}} + \text{OH} \rightarrow \text{CO} + \frac{1}{2}\text{H}_2$
8. $\text{C}_2\text{H}_2 + \text{O}_2 \rightarrow 2\text{CO} + \text{H}_2$
9. $R + \text{O}_2 \rightarrow \text{product}$
Spatial soot contours

Estimated $\phi$ at lift-off

PLII (Sandia)

$1000 \text{ K}$
$\phi(H) = 3.4$

$900 \text{ K}$
$\phi(H) = 2.0$

$850 \text{ K}$
$\phi(H) = 1.4$

Distance from injector [mm]

Lift-off varying Tamb @ 3.2 ms

Predicted $\phi$ at lift-off

Predicted soot mass fraction

Sooting: $Y_{\text{soot}} \sim 1.0E-5$
Non-sooting: $Y_{\text{soot}} \sim 1.0E-8$

Soot

$3.50E-5$
$1.75E-5$
$0.00E-5$

DEER-2005
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
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

- **Solid Line**: Experimental
- **Broken Line**: Simulated

### Graph
- **Pressure (MPa)** vs. **CAD ATDC**

### Table
<table>
<thead>
<tr>
<th></th>
<th>High-T Short-ID - Diffusion combustion</th>
<th>High-T, Long-ID - Premixed combustion</th>
<th>Low-T, Early-Inj. (Lean Premixed)</th>
<th>Low-T, Late-Inj. (MK)</th>
<th>Low-T, Double-Inj. (UNIBUS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Speed (RPM)</td>
<td>1200</td>
<td>1200</td>
<td>1200</td>
<td>1200</td>
<td>1200</td>
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<tr>
<td>IMEP (bar)</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>4</td>
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<tr>
<td>Injection Pressure (bar)</td>
<td>1200</td>
<td>1200</td>
<td>1600</td>
<td>1600</td>
<td>1600</td>
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<tr>
<td>Intake Temp (°C)</td>
<td>111</td>
<td>47</td>
<td>90</td>
<td>70</td>
<td>90</td>
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<tr>
<td>Intake Pressure (kPa)</td>
<td>233</td>
<td>192</td>
<td>214</td>
<td>202</td>
<td>214</td>
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<tr>
<td>TDC Motored Temp. (K)</td>
<td>900</td>
<td>750</td>
<td>867</td>
<td>819</td>
<td>867</td>
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<td>TDC Mot. Density (kg/m³)</td>
<td>24</td>
<td>24</td>
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<td>24</td>
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<tr>
<td>SOI (°ATDC)</td>
<td>-7</td>
<td>-5</td>
<td>-22</td>
<td>0</td>
<td>-22, +15</td>
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<td>Injection Quantity (mg)</td>
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<td>61</td>
<td>56</td>
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<td>31, 33</td>
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<td>DOI (CAD)</td>
<td>10</td>
<td>10</td>
<td>7</td>
<td>7</td>
<td>4, 4</td>
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<tr>
<td>O₂ Conc. (Vol %)</td>
<td>21</td>
<td>21</td>
<td>12.6</td>
<td>12.6</td>
<td>12.6</td>
</tr>
</tbody>
</table>

**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

- 821 rpm, 25% load cooled EGR

Highly premixed combustion characteristics

8% EGR

40% EGR
ERC Caterpillar NOx & Soot emission predictions

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

**NOx Emission vs. SOI**

**Soot emission vs. SOI**
Model application - Diesel LTC challenges

- **Vaporization too slow**
  - 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

- **Ignition too fast**
  - 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

- Tradeoff
- 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

GA optimized low pressure injection

Two-Pulse Sprays
Variable geometry sprays

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

SOI = -143 deg ATDC
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)