On-line diagnostics and fast modeling of soot formation / oxidation in diesel engine combustion

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At the Aerothermochemistry and Combustion Systems Laboratory of the Swiss Federal Institute of Technology in Zurich we are currently developing low emissions strategies for heavy-duty diesel engines that engine manufacturers can implement to meet stringent emissions regulations. The technologies being studied include high-pressure fuel injection (with common-rail injection system), turbocharging, and exhaust gas recirculation (cooled EGR). We also investigate the influence of oxygenated diesel fuel additives and water-diesel fuel emulsions on combustion and emissions [1]. Measurements are carried out on a heavy-duty four-cylinder diesel engine equipped with turbocharger and common-rail fuel injection. Wide variations of injection parameter settings and EGR rate are performed. Engine experiments are conducted with reference diesel fuel and 3 different water-diesel fuel emulsions (13% / 21% / 30% Water) and with a blend of reference diesel fuel and butyal. The experimental study includes measurements of pollutants in the exhaust gas (Opacity, Filter Smoke Number, Particulate Number Size Concentration, gaseous components as NOx, HC ...) as well as in-cylinder on-line measurements of soot concentration / soot temperature by means of the two-color pyrometry method.

An optical probe developed by Schubiger in 2001 [2] is used to collect the light intensity of the soot radiation during combustion. The soot concentration (KL-factor) and the transient burned gas temperature are computed with the multicolour-pyrometry technique (3 wavelengths). The measurements show that the KL-signal start coincides with the beginning of the mixing-controlled combustion phase where soot is first formed. The soot formation and oxidation processes are clearly recognizable form the KL-data plots over time. The measured transient burned gas temperature reaches a maximum at the occurrence of “injection process ends”. A match of the measured burned gas temperature with a computed temperature in the combustion chamber obtained by varying the air/fuel ratio (A/F) in the 2-zone model, shows that the local A/F during soot formation starts at 0.55 (fuel rich) and ends up at ca. 0.9 (near stoichiometric) at the end of the soot oxidation phase.

The variation of the fuel composition (use of water-diesel fuel emulsions or oxygenated diesel additives) leads to reduced soot formation rate and enhanced soot oxidation rate. Moreover, at higher injection pressures there is clear indication that the soot oxidation process begins earlier and is more effective. The measured soot radiation temperature is lower when using water-diesel fuel emulsions respectively abot the same as that of the reference diesel fuel when using oxygenated diesel additives. The exhaust gas recirculation lowers the soot oxidation process dramatically, this fact is responsible for having higher particulate emissions at higher EGR rates. Data of in-cylinder soot concentration at the end of the soot oxidation phase (KL-factor after the drop passed the second KL-maximum) correlate clearly with particulate measurements in the exhaust (total number of particles 20-500 nm and filter smoke number) [3].
The LAV approach for fast modeling of soot formation / oxidation processes during the combustion is accomplished with phenomenological models (0-D fast modeling) and with 3D-simulations. It is based on a simplified and essentially correct description of the physical and chemical mechanisms prevailing in diesel engine combustion. The approach includes submodels for the prediction of heat release rate, NO and soot emissions [2, 4]. The model parameters (ca. 10 for the soot model) are identified and optimized with bioinspired evolutionary algorithms (stochastic, parallel search method) using typically 20 engine measurements with a wide range of operating conditions [4]. The model validation carried out for different engine operating conditions shows very promising results; the model can predict the particulate emissions of diesel engines with high accuracy and in short time. It is for example possible to compute 1Mio operating conditions in the engine map within 2 days using 3 PC's, while for the same task the optimization of PM emissions at the engine test bench would take 1000 times more.

Conclusions and outlook:
- Particle number size measurements in the exhaust gas have been combined with relevant combustion parameters and in-cylinder measurements of soot concentration.
- The combination of a flexible -high pressure- fuel injection system, exhaust gas recirculation, oxygenated fuels and water-diesel fuel emulsion technology allowed to separate important thermochemical and fluidmechanical influences.
- Soot measurements in the combustion chamber and in the exhaust were used for the development and the validation of phenomenological soot models which can help to optimize the diesel engine combustion process in shorter time.

References:
Research approach & motivation

Exhaust emissions

Heavy-duty diesel engine common rail injection system

Fuel-related parameters
- Fuel injection
- Fuel composition
Air-related parameters
- Exhaust gas recirculation
- Turbocharging

Combustion analysis & Modeling of soot formation/oxidation

Crank angle-resolved data of in-cylinder soot concentration
Heavy-Duty Diesel Engine

- **LIEBHERR 4-cylinder 4-stroke direct injected diesel engine**
  - Stroke = 142 mm; Bore = 122 mm
  - \( V_e = 6.64 \, l \); \( \varepsilon = 17.2 \)
  - 183 kW @ 2100 1/min
  - 1060 Nm @ 1540 1/min

- **Common Rail Injection System**
  - ETH pump (-2000 bar)
  - BSG electronic (main, pilot & post injection)
  - CRT injectors (-1600 bar), Type P2
  - Bosch injectors (-1200 bar)
  - Nozzle tips 6*0.210, 8*0.200 mm

- **Turbocharger**
  - Compressor K 27.2 (original)
  - Turbine casings T21, T15, T12

- **EGR-System (preliminary)**
  - Cooled EGR (high pressure side)
  - With throttle after turbine
## Fuel properties

<table>
<thead>
<tr>
<th></th>
<th>Water content $m_W/(m_D+m_A)$ [%]</th>
<th>Oxygen Content $m_{O_2}/m_{tot}$ [%]</th>
<th>Lower heating value [MJ/kg]</th>
<th>Density [kg/m³]</th>
<th>Stoichiometric air/fuel ratio [-]</th>
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<tbody>
<tr>
<td>Reference diesel</td>
<td>0</td>
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<td>43.14</td>
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<tr>
<td>13% W-D emulsion</td>
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<td>21% W-D emulsion</td>
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<td>15.36</td>
<td>34.96</td>
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<td>30% W-D emulsion</td>
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<td>20.6</td>
<td>32.54</td>
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<tr>
<td>60% butylal blend</td>
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<td>11.98</td>
<td>38.25</td>
<td>829</td>
<td>12.57</td>
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</table>
Diagnostics on a HD diesel engine
Optical in-situ soot observation; multi-colour pyrometry

Sensor position
(field of view, „measuring volume“)

Sensor position within the cylinder head

Source: R Schubiger 2001
Optical lightwaveguide diagnostics

Source: R Schubiger 2001
On-line, global information on soot concentration and (radiation) temperature

Reference diesel fuel, 1250 rpm, 10 bar BMEP, p rail 800 bar, SOI 1°CA ATDC
Multi-colour pyrometry
variation of fuel composition and injection parameters

Constant Injection Pressure
- Ref. Diesel, pRail 800 bar
- 13% Water Em., pRail 800 bar
- 30% Water Em., pRail 800 bar
- 60% Butylal Bl., pRail 800 bar

Burn Rate
\( \frac{dQ}{d\phi} [J/°CA] \)

KL-Factor [\(-\)]

Measured Temperature [K]

Crank angle degrees

Constant Injection Duration
- Ref. Diesel, pRail 800 bar
- 13% Water Em., pRail 940 bar
- 30% Water Em., pRail 1060 bar
- 60% Butylal Bl., pRail 940 bar

Burn Rate
\( \frac{dQ}{d\phi} [J/°CA] \)

KL-Factor [\(-\)]

Measured Temperature [K]

Crank angle degrees
Multi-colour pyrometry
Variation of fuel composition and EGR rate

- Ref. Diesel, no EGR
- Ref. Diesel, 12.6% EGR
- 30% Water Em., no EGR
- 30% Water Em., 12.6% EGR

Burn Rate $\frac{dQ}{d\phi} [\text{J/°CA}]$

KL-Factor [-]

Measured Temperature [K]

Crank angle degrees
Results: influence of fuel composition

Engine speed 1250 rpm, 50% load
Injection strategy D
Injection pressure: 800 bar (diesel) - 970 (21% em) - 1050 bar (30% em) - 930 bar (60% butylal)
Fundamentals

Boulouchos et al. (2001)\(^1\)


3 Basic Equations (Formation, Oxidation & Sum-up)
Dimensional Correct Formulation
Oxidation $\sim$ Inverse Characteristic Mixing-Time

Akihama et al. (2001)\(^2\)


„Φ-T diagram“ for soot formation
Basis: CHEMKIN „stirred reactor“ calculations
(including PAH formation, soot particle nucleation, coagulation, growth and surface reactions)
„ETH-LAV“ approach – concept

Settings

„Basic“ Principles of Physics & Chemistry

Aim: Computing Times « 3D-CRFD
Accuracy » Empirical Models

Approach

Phenomenological Models

Dimension adjusted Equations
Elementary Physics & Chemistry included

Parameterization

Evolutionary Algorithms
No Dependency on Operating Conditions (!)

Validation / Application

Different Engine Set-Ups
\( V_d = 0.5 .. 1000 \text{ [l/cyl]} \)

Chemistry

\[
\frac{dm_{\text{Fuel Diff}}}{dt} = \frac{1}{\tau_{\text{Diff}}} \cdot m_{\text{Fuel Evap}}
\]

Physics

(Diffusion Flame)

Efficient Phenomenological Models

Mutation
Recombination
Selection
Fitness Evaluation

(Re-parameter Optimization with Evolutionary Algorithms)
Example – soot emissions – parameter identification

**Engine**
- 4-cyl. CR-DI Diesel
  \( V_d \approx 1.6 \text{ [l]} \)

- \( n \) 1250 .. 1830 [min\(^{-1}\)]
- \( p_{\text{me}} \) 3.7 .. 14 [bar]
- \( p_{\text{inj}} \) 400 .. 1400 [bar]
- \( \text{SOI} \) -14 .. 0 [°CA aTDC]
- \( \text{EGR} \) 0 .. 30 [%]

**PM \text{ [g/kWh]}**

<table>
<thead>
<tr>
<th>Operating Conditions ([-])</th>
<th>Simulation</th>
<th>Experiment</th>
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**Accuracy of measurements**
Example – soot emissions – model validation

Engine
4-cyl. CR-DI Diesel
\( V_d \approx 1.6 \,[\text{l}] \)

Range of Op. Conditions
- \( n \)
  \( 1250 \ .. \ 1830 \,[\text{min}^{-1}] \)
- \( p_{\text{me}} \)
  \( 4.0 \ .. \ 16 \,[\text{bar}] \)
- \( p_{\text{inj}} \)
  \( 350 \ .. \ 1600 \,[\text{bar}] \)
- SOI
  \( -12 \ .. \ 3 \,[^\circ\text{CAaTDC}] \)
- EGR
  \( 0 \ .. \ 43 \,[\%] \)

Accuracy of measurements
Conclusions and outlook

- Particle number size measurements in the exhaust gas have been combined with relevant combustion parameters and in-cylinder measurements of soot concentration.

- The combination of a flexible -high pressure- fuel injection system, exhaust gas recirculation, oxygenated fuels and water-diesel fuel emulsion technology allowed to separate important thermochemical and fluidmechanical influences.

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