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

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8 ETH Conference on combustion generated nanoparticles
August 16, 2004

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 butylal.
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:

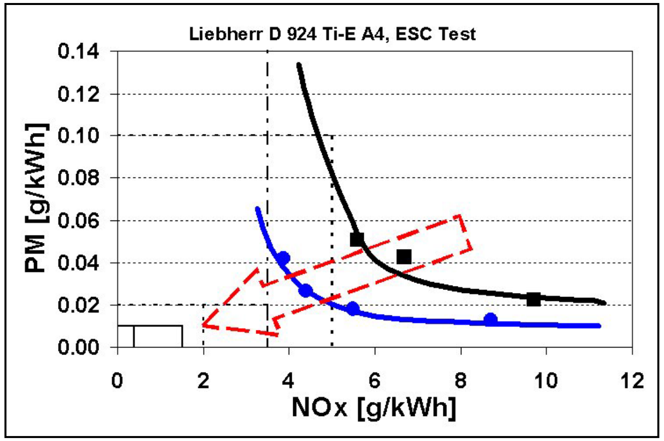
- Particle number size measurements in the exhaust gas have been combined with relevant combustion parameters and in-cylinder measurements of soot concentration.
- The combination of a flexible -high pressure- fuel injection system, exhaust gas recirculation, oxygenated fuels and water-diesel fuel emulsion 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.

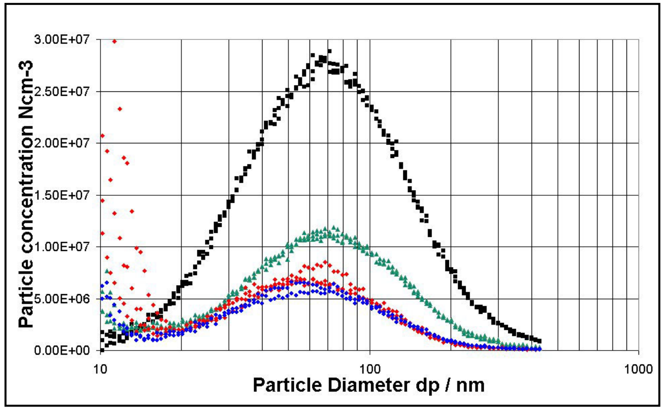
References:

[1] Bertola A : *Technologies for Lowest NOx and Particulate Emissions in DI-Diesel Engine Combustion - Influence of Injection Parameters, EGR and Fuel Composition*, Thesis dissertation ETH Zurich nr.15373, 2003.
[2] Schubiger S : *Untersuchungen zur Russbildung und -oxidation in der dieselmotorischen Verbrennung: Thermodynamische Kenngrössen, Verbrennungsanalyse und Mehrfarbenendoskopie,* Thesis dissertation ETH Zurich nr.14445, 2002.
[3] Bertola A et al : *Temporal Soot Evolution in Diesel Engine Combustion – Influence of Fuel Composition, Injection Parameters and EGR*, 2004 in preparation.
[4] Warth M et al: *Prediction of Heat Release Rates, NO- and Soot Emissions in Diesel-Engines – Optimization and Validation of a New Approach,* 9th Symposium "The Working Process of the Internal Combustion Engine", Institute for Internal Combustion Engines and Thermodynamics, Graz University of Technology, 2003.

Research approach & motivation

Exhaust emissions





Heavy-duty diesel engine common rail injection system

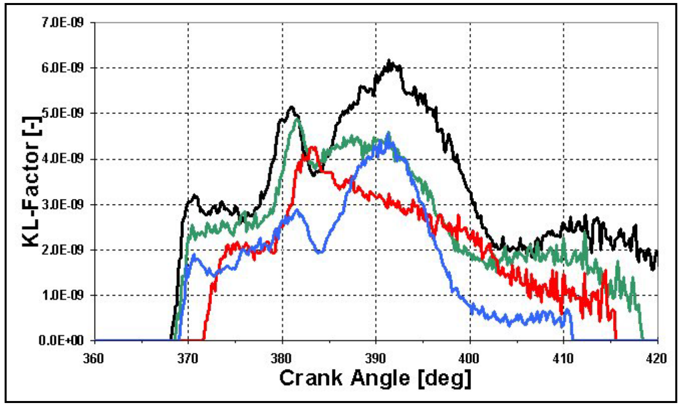
Fuel-related parameters

- Fuel injection
- Fuel composition

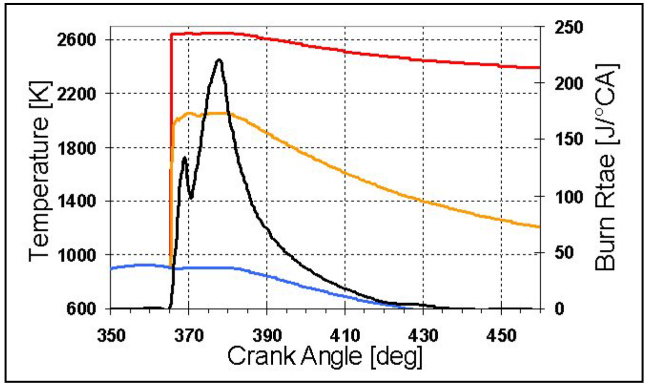
Air-related parameters

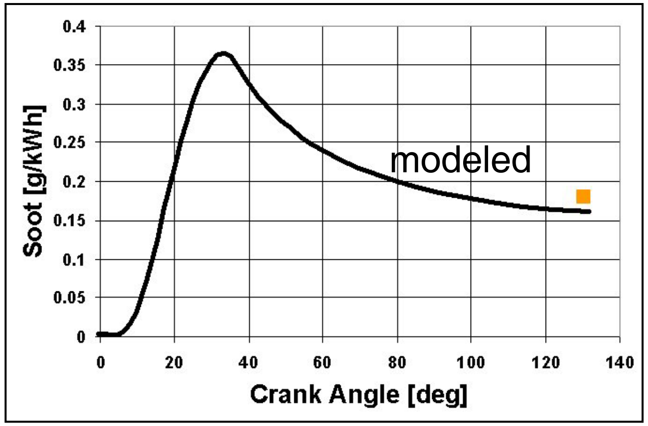
- Exhaust gas recirculation
- Turbocharging

Crank angle-resolved data of in-cylinder soot concentration

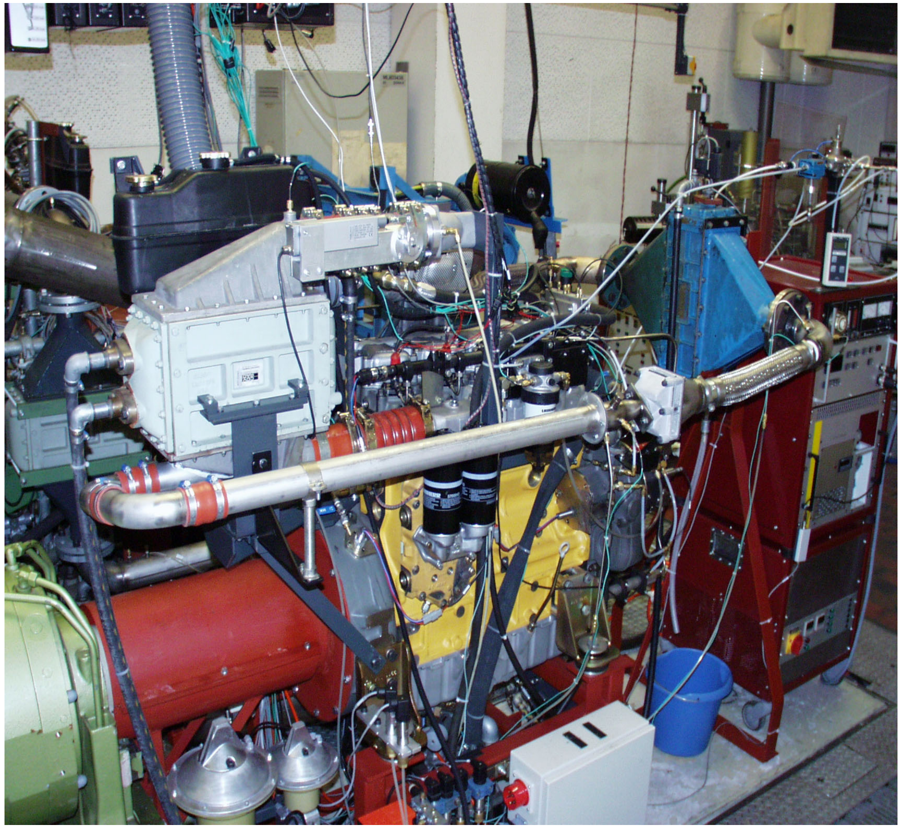


Combustion analysis & Modeling of soot formation/oxidation





Heavy-Duty Diesel Engine



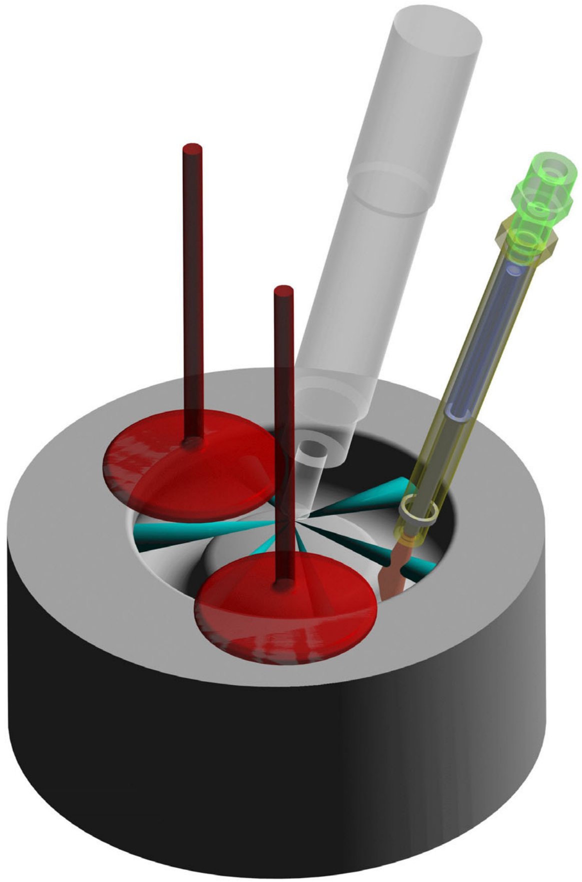
- **LIEBHERR 4-cylinder 4-stroke direct injected diesel engine**
  - Stroke = 142 mm; Bore = 122 mm
  - V_e = 6.64 l ; ε = 17.2
  - 183 kW @ 2100 1/min
  - 1060 Nm @ 1540 1/min
- **Common Rail Injection System**
  - ETH pump (-2000 bar)
  - BSG electronic (main, pilot & post injection)
  - CRT injectors (-1600 bar), Type P2
  - Bosch injectors (-1200 bar)
  - Nozzle tips 6*0.210, <u>8*0.200</u> mm
- **Turbocharger**
  - Compressor K 27.2 (original)
  - Turbine casings T21, <u>T15</u>, T12
- **EGR-System (preliminary)**
  - Cooled EGR (high pressure side)
  - With throttle after turbine

Fuel properties

	Water content $m_W/(m_D+m_A)$	Oxygen Content m_{O2}/m_{tot}	Lower heating value	Density	Stoichiometric air/fuel ratio
	[%]	[%]	[MJ/kg]	[kg/m3]	[-]
Reference diesel	**0**	**0**	**43.14**	**819**	**14.64**
13% W-D emulsion	**13**	**10.15**	**37.98**	**851**	**12.98**
21% W-D emulsion	**21**	**15.36**	**34.96**	**862**	**12.38**
30% W-D emulsion	**30**	**20.6**	**32.54**	**871**	**11.77**
60% butylal blend	**0**	**11.98**	**38.25**	**829**	**12.57**

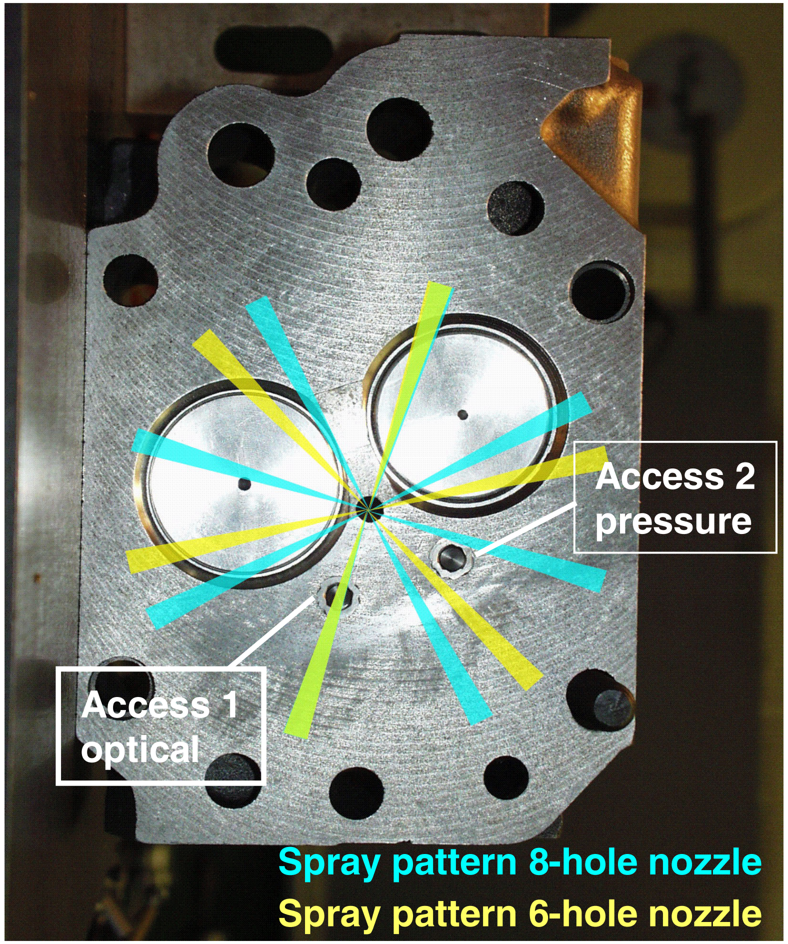
Diagnostics on a HD diesel engine
Optical in-situ soot observation; multi-colour pyrometry

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

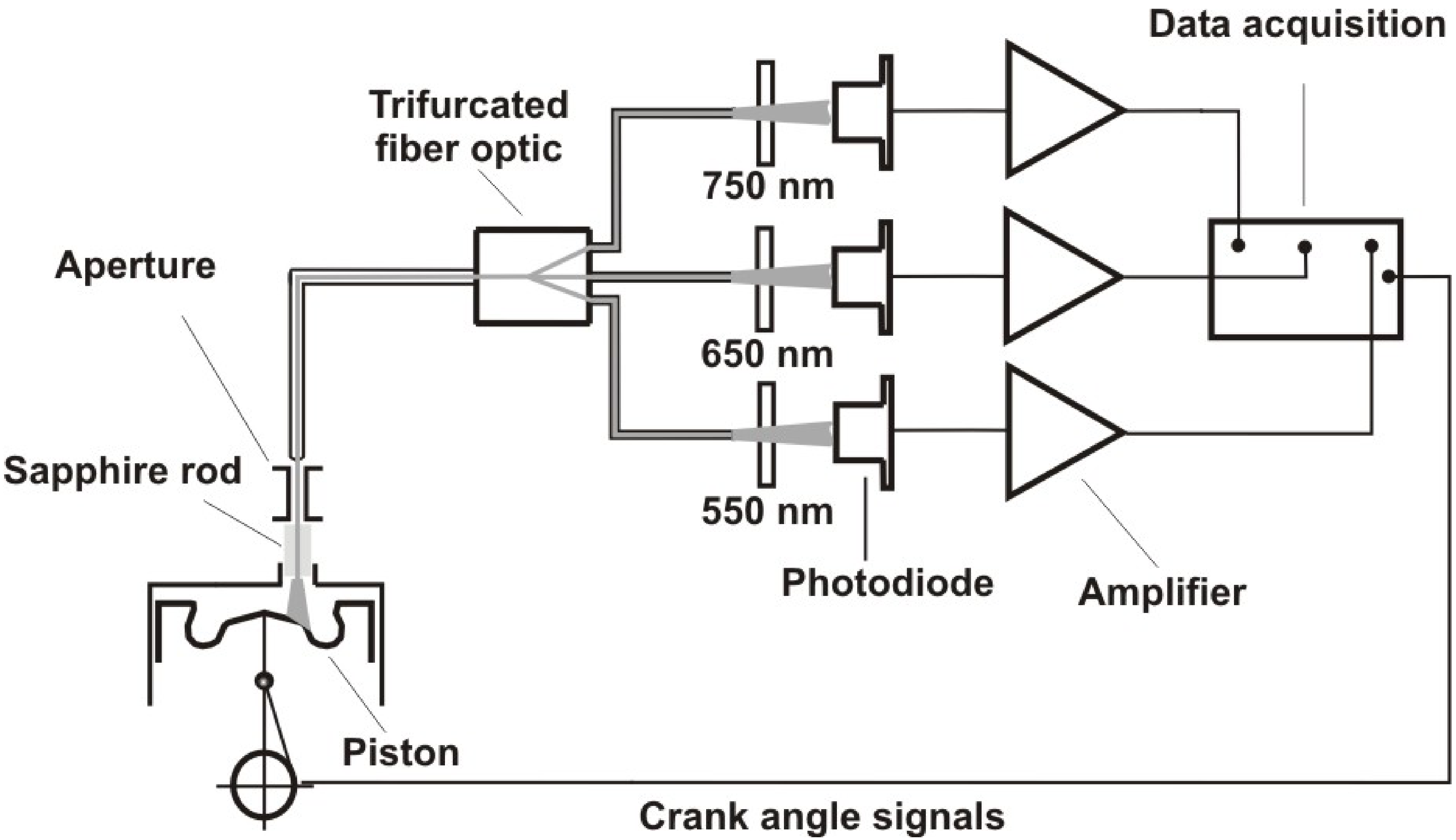


Source: R Schubiger 2001

Sensor position within the cylinder head



Optical lightwaveguide diagnostics



Source: R Schubiger 2001

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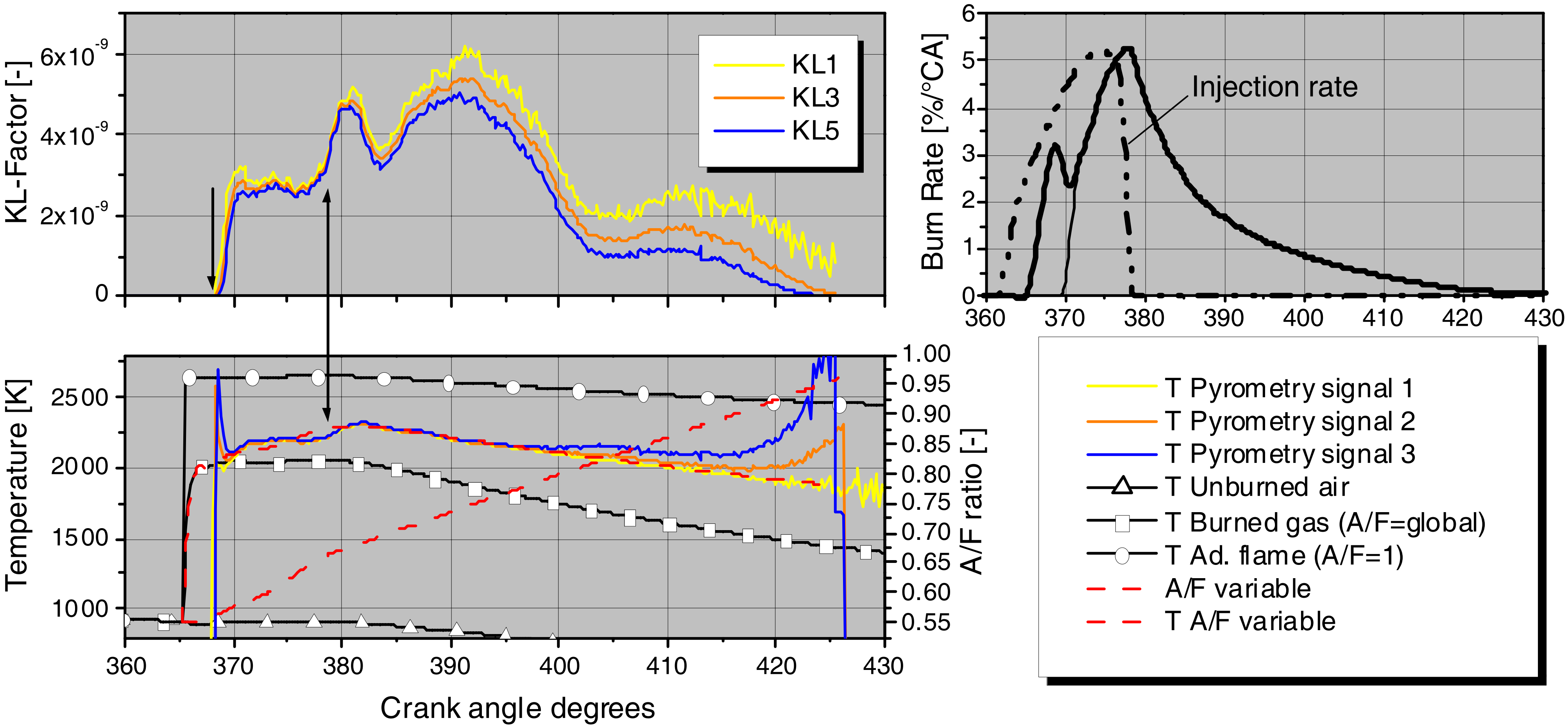
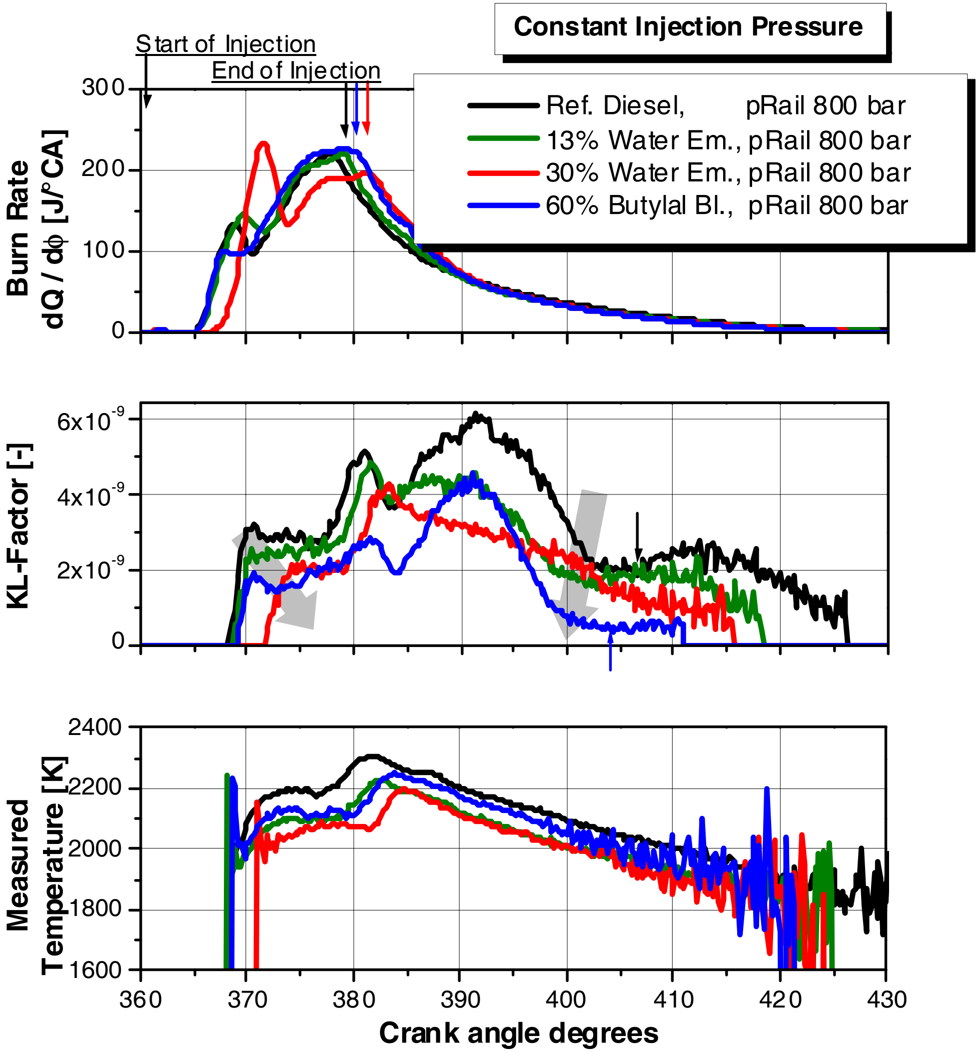
LAV

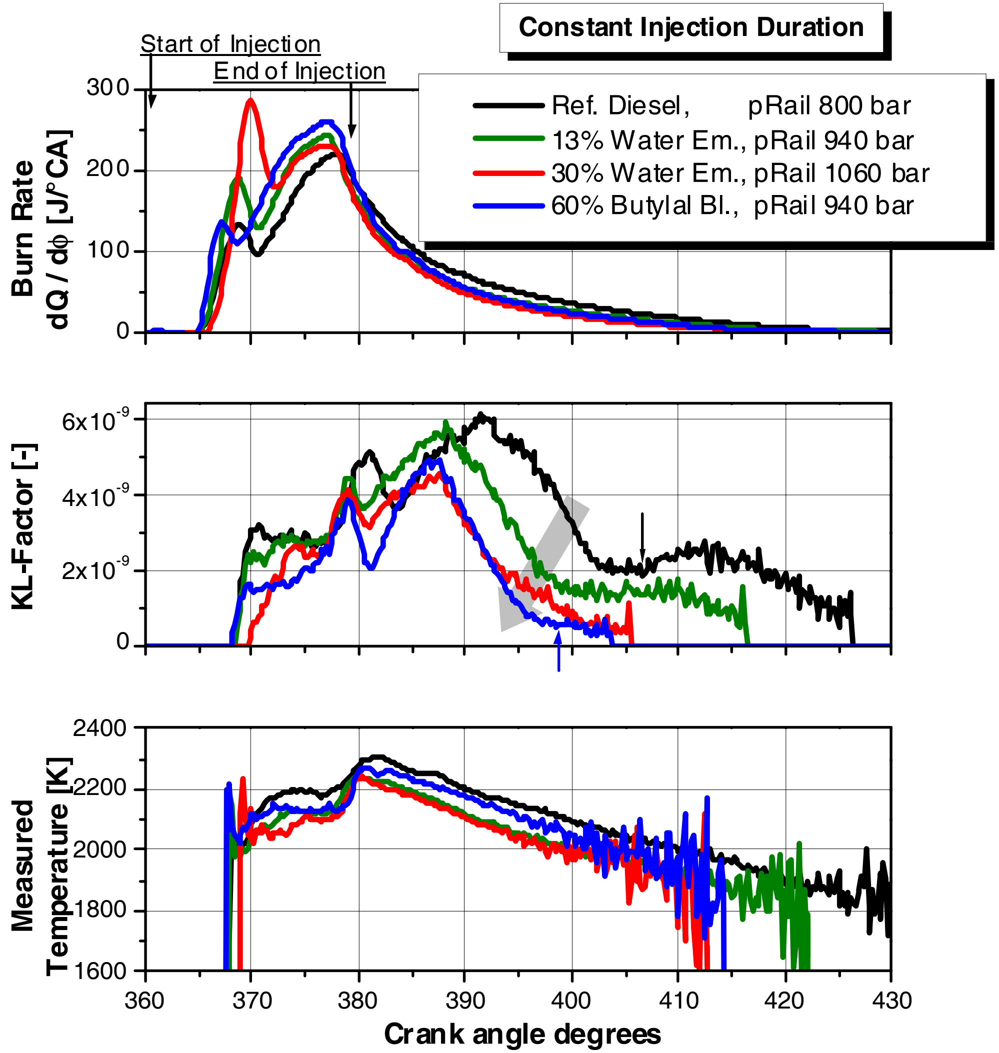
On-line, global information on soot concentration and (radiation) temperature



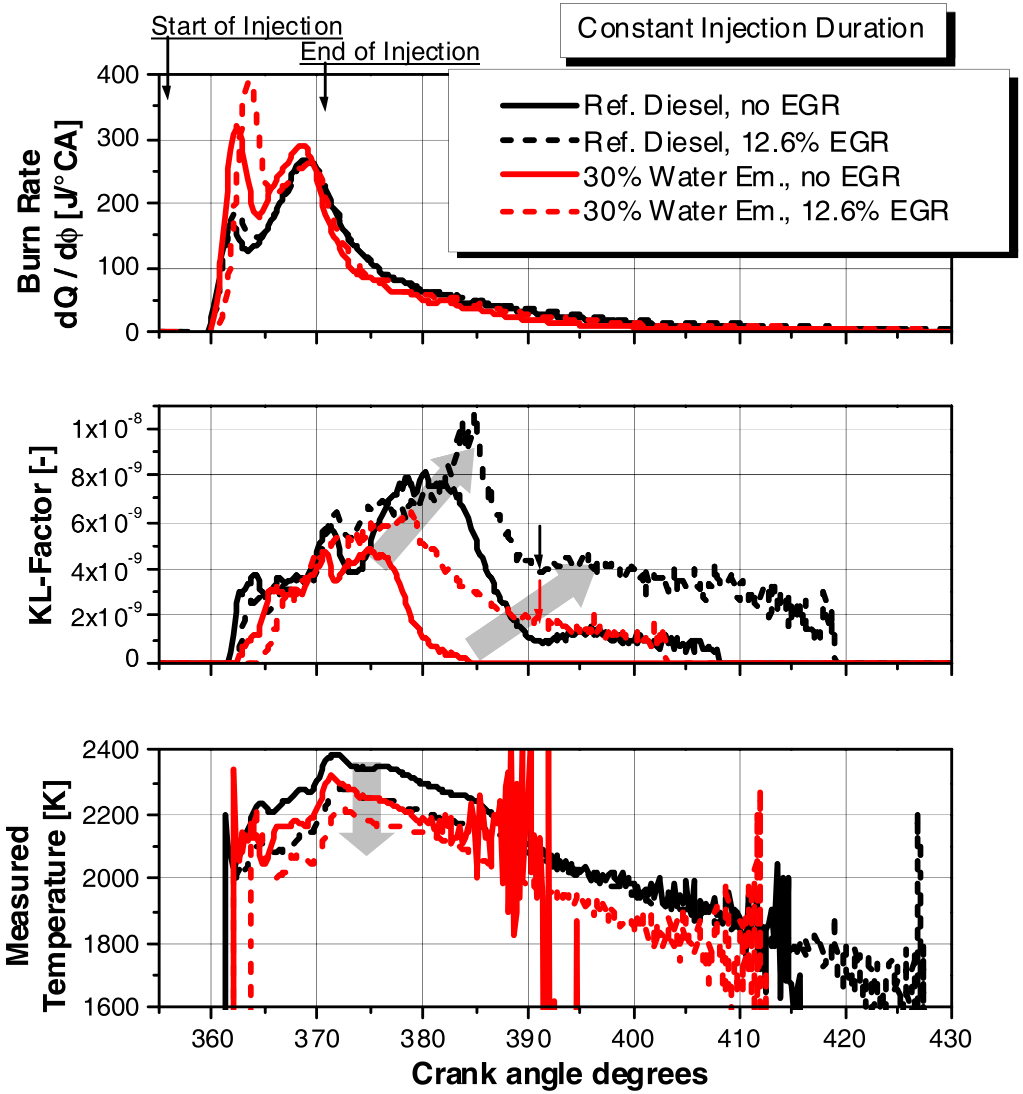
Reference diesel fuel, 1250 rpm, 10 bar BMEP, p rail 800 bar, SOI 1°CA ATDC

Multi-colour pyrometry
variation of fuel composition and injection parameters



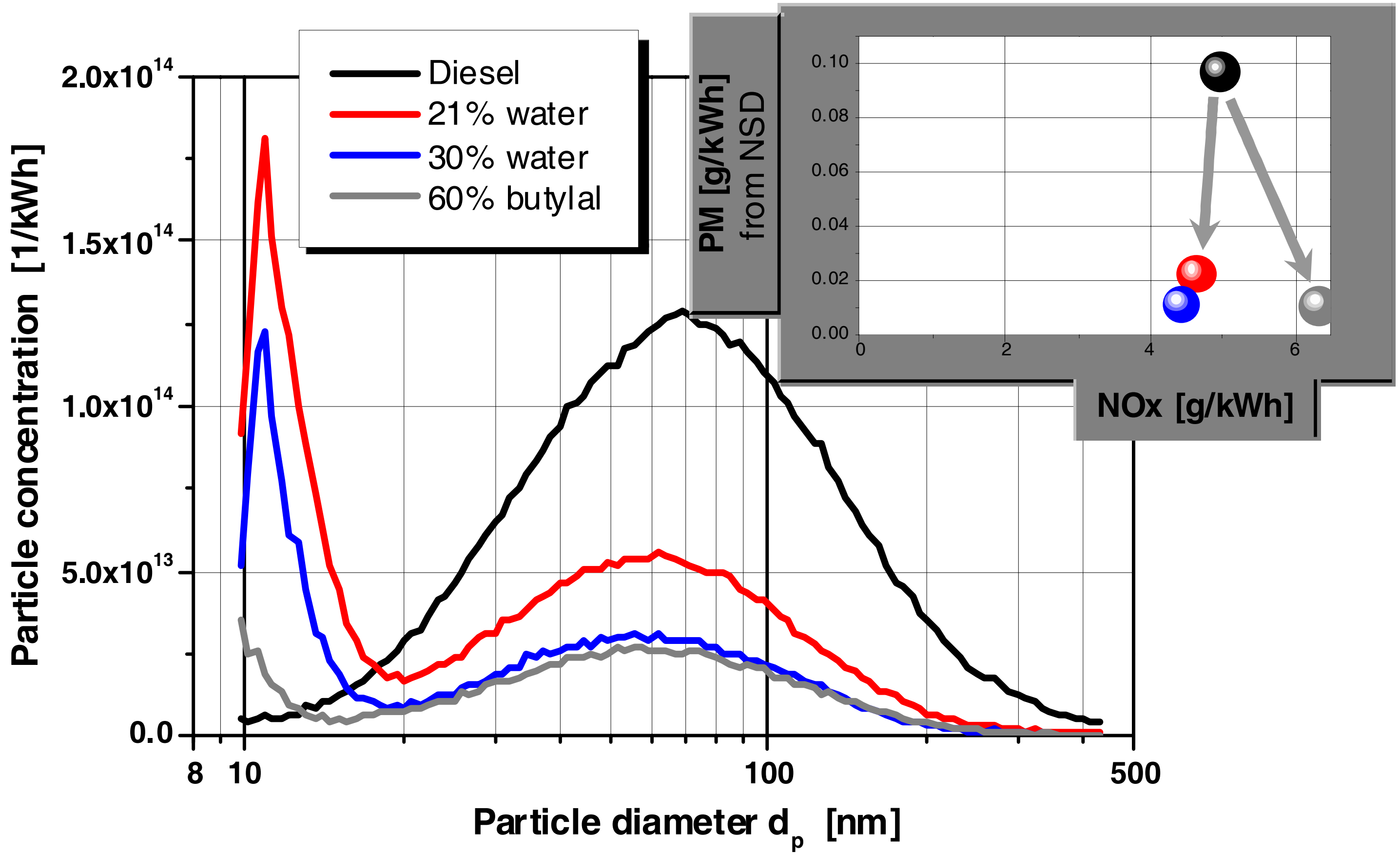


Multi-colour pyrometry
Variation of fuel composition and EGR rate



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)



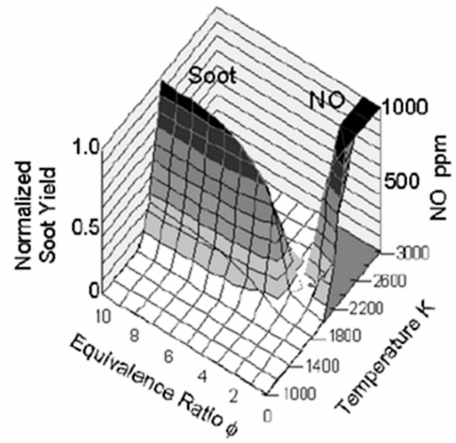
„ETH-LAV“ approach – soot modeling

Fundamentals

Boulouchos et al. (2001)[1]

[1] Schubiger, R. et al. *Russbildung und Oxidation bei der dieselmotorischen Verbrennung*. MTZ 5/2002 (63), pp. 342-353.

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

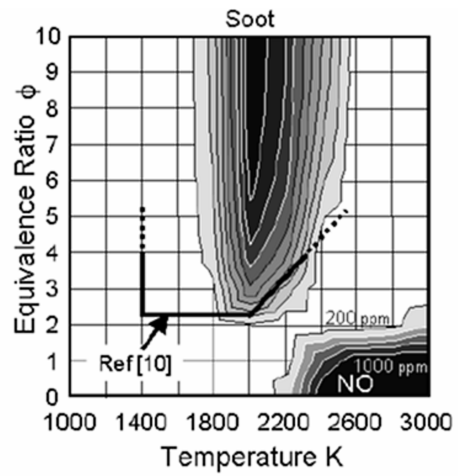


Based on detailed CHEMKIN calculations

Akihama et al. (2001)[2]

[2] Akihama, K. et al. *Mechanism of the smokeless rich diesel combustion by reducing temperature*. SAE 2001-01-0655, Warrendale, PA, USA, 2001.

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



Source: Akihama et al.

„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

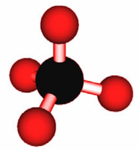
No Dependency on Operating Conditions (!)

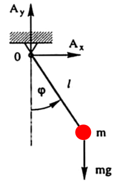
Validation / Application

Different Engine Set-Ups

($V_d = 0.5 .. 1000$ *[l/cyl]*)

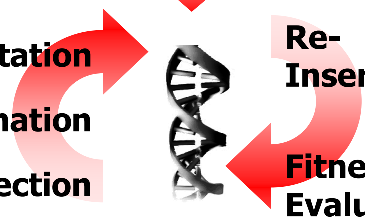
Chemistry **Physics**





$$\frac{dm_{Fuel\ Diff}}{dt} = C \cdot \frac{1}{\tau_{Diff}} \cdot m_{Fuel\ Evap}$$

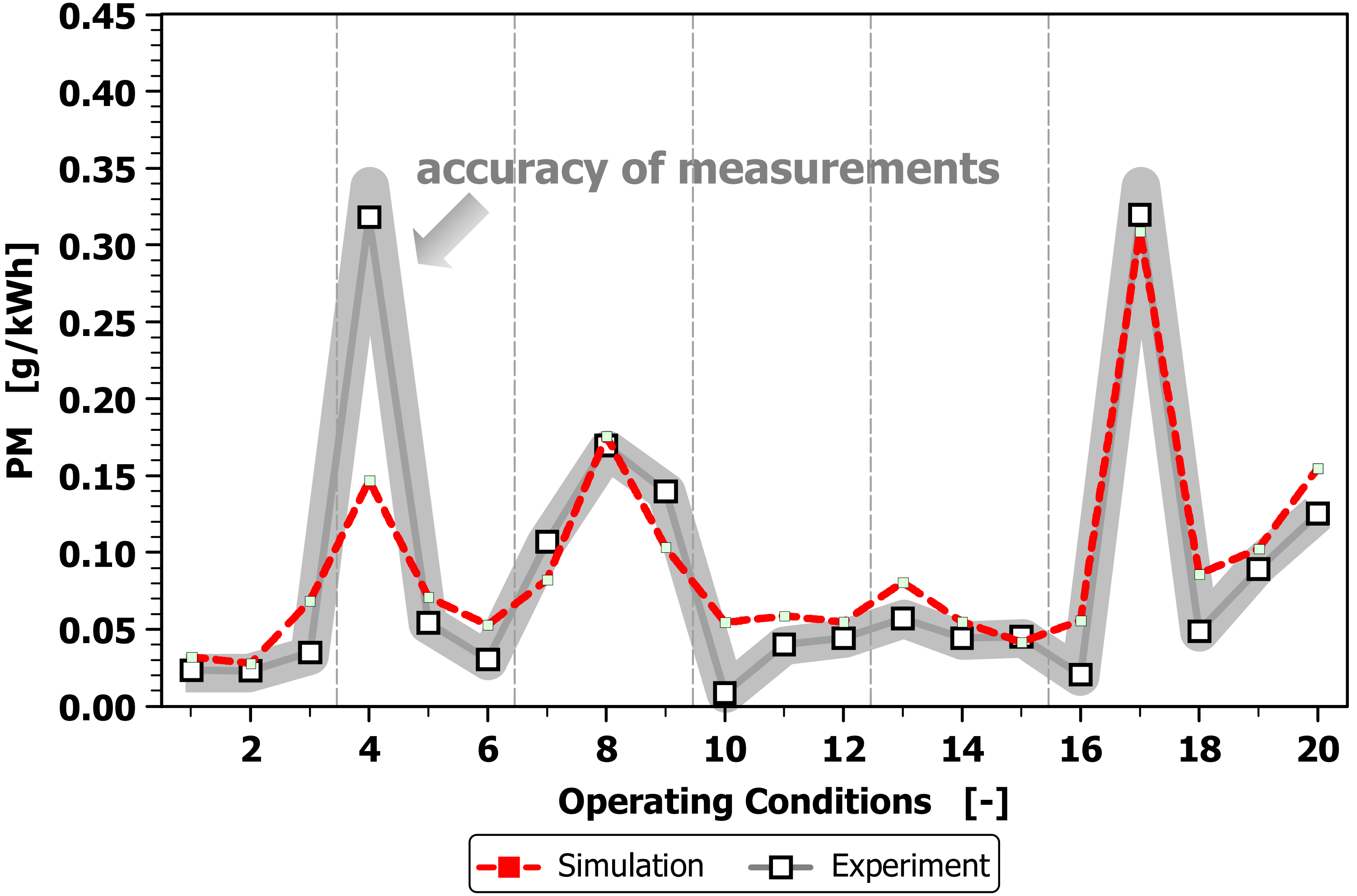
(Diffusion Flame)



(Parameter Optimization with Evolutionary Algorithms)

Efficient Phenomenological Models

Example – soot emissions – parameter identification



Engine

4-cyl. CR-DI Diesel
($V_d \approx 1.6$ [l])

Range of Op. Conditions

n
1250 .. 1830 [min^{-1}]

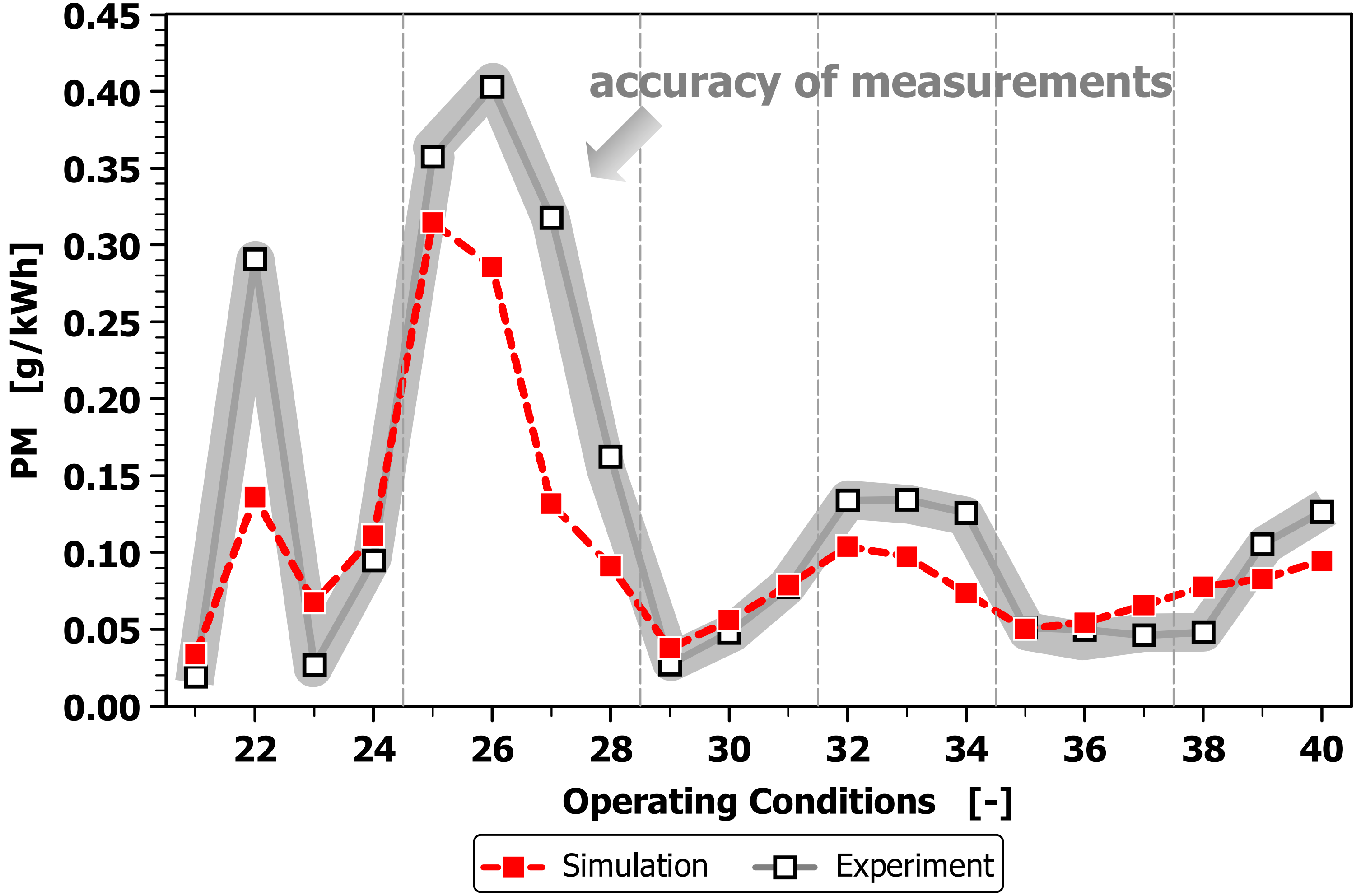
p_{me}
3.7 .. 14 [bar]

p_{inj}
400 .. 1400 [bar]

SOI
-14 .. 0 [°CA aTDC]

EGR
0 .. 30 [%]

Example – soot emissions – model validation



Engine

4-cyl. CR-DI Diesel
($V_d \approx$ 1.6 [l])

Range of Op. Conditions

n
1250 .. 1830 [min^{-1}]

p_{me}
4.0 .. **16** [bar]

p_{inj}
350 .. **1600** [bar]

SOI
-12 .. **3** [°CA aTDC]

EGR
0 .. **43** [%]

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

Acknowledgements

M. Mohr and U. Mathis (EMPA)

Swiss Federal Office of Energy (BFE)

LIEBHERR Machines Bulle S.A.

Common Rail Technologies AG

Lubrizol Corporation

Lambiotte & Cie S.A.