Bio-Fuel research at Chalmers

Ingemar Denbratt

Background

- There is a need to reduce the dependence of fossil fuels due to:
  - Global warming
  - Finite resources
- The fossil fuels will be gradually replaced
- There will not be just one alternative
- Viable alternatives must be found and evaluated
- Qualification criteria's:
  - Environmental impact
  - Efficiency
  - Production cost

Fuels for CI engines studied at Chalmers:

- FAME fuels (RME, SME and PME)
- DME
- Dual-Fuel (Diesel/Nat. Gas)

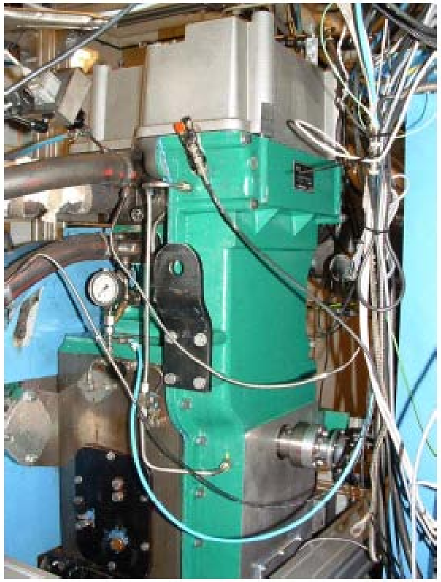
Both experiments and simulations have been performed

FAME
(RME, SME and PME)

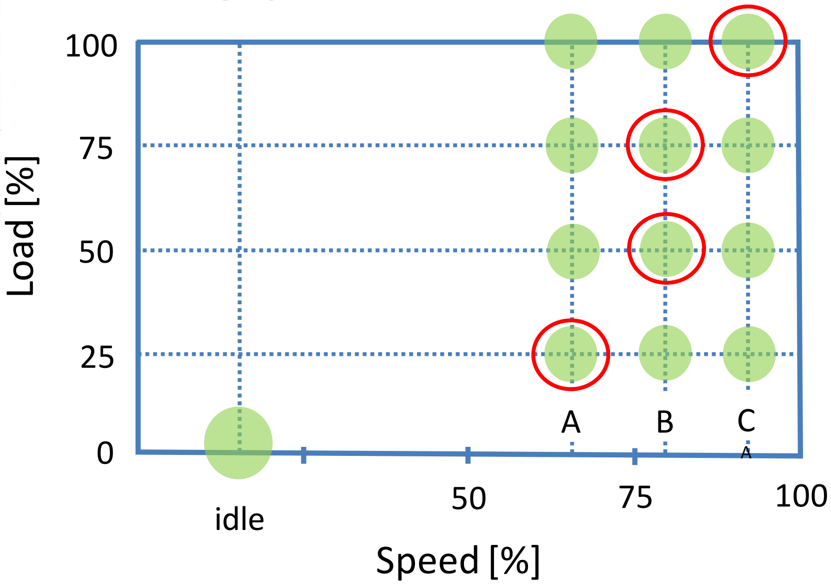
Monica Johansson, Junfeng Yang, Valeri Golovitchev and Ingemar Denbratt

	Methods	Unit	EN590 (EU diesel)	RME	SME	PME
Density	D-4052	Kg/m3	840,9	883,3	885,6	874,5
Sulfur	D-5453	mg/kg	23			
Aromatics	D-6591	Weight %	24,3	NA	NA	NA
Flash point	D-93	Deg C	73	154	159	172
CFPP	IP 309	Deg C	-29	-16	-3	13
Viskosity @ 40 deg C	D-445	mm2/s	2,713	4,468	4,215	5,136
Cetane nr	D-613		52,8	53,4	50,4	61,1
Heating value (net)			42,8	37,34	37,32	36,96
Carbon	D-5291	Weight %		77,5	77,3	76,8
Hydrogen	D-5291	Weight %		12,2	11,9	12,6
Oxygen	CHNS-O	Weight %		10,0	9,8	7,6
IBP	D-86	Deg C	184,8	317	321	315
FBP	D-86	Deg C	334	346	337	344
Oxidation stability	EN 15751	h		8,7	5,7	6,8

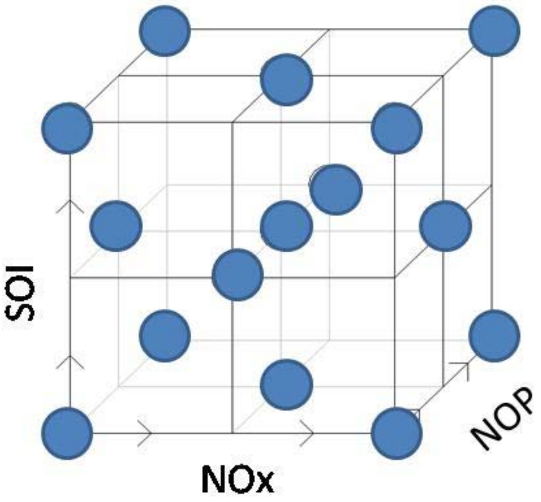
Experiments



ESC

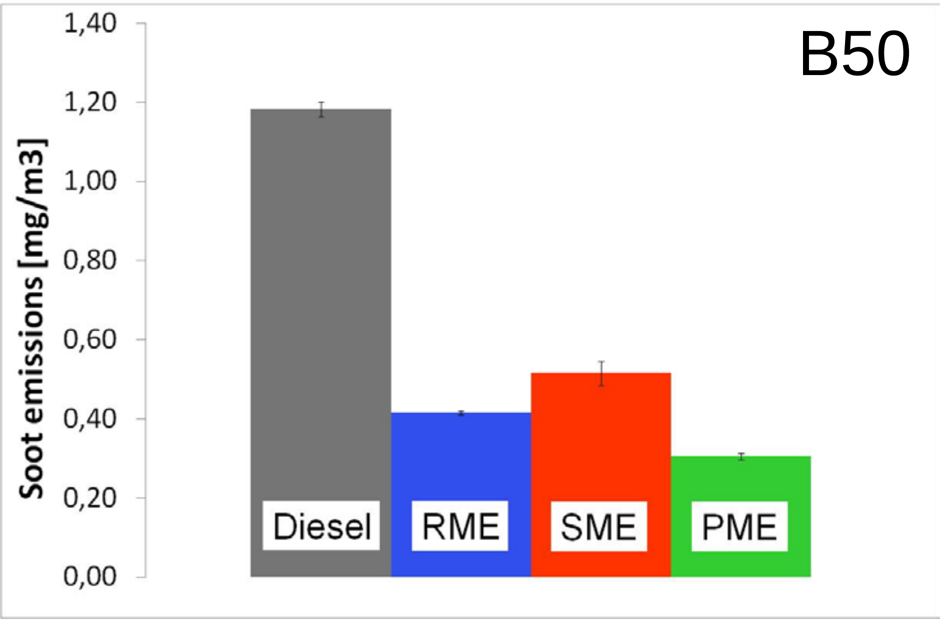


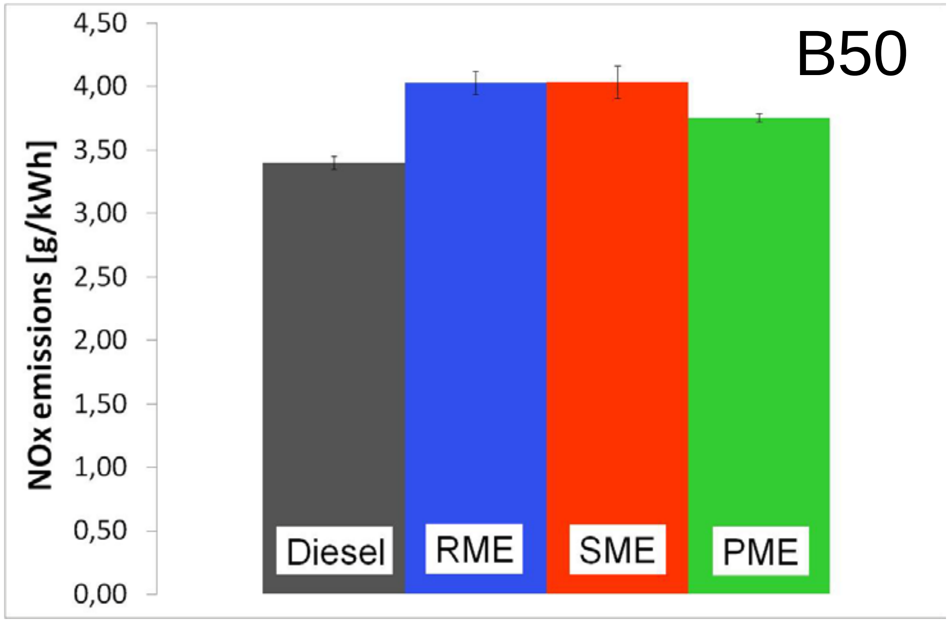
DOE for A25



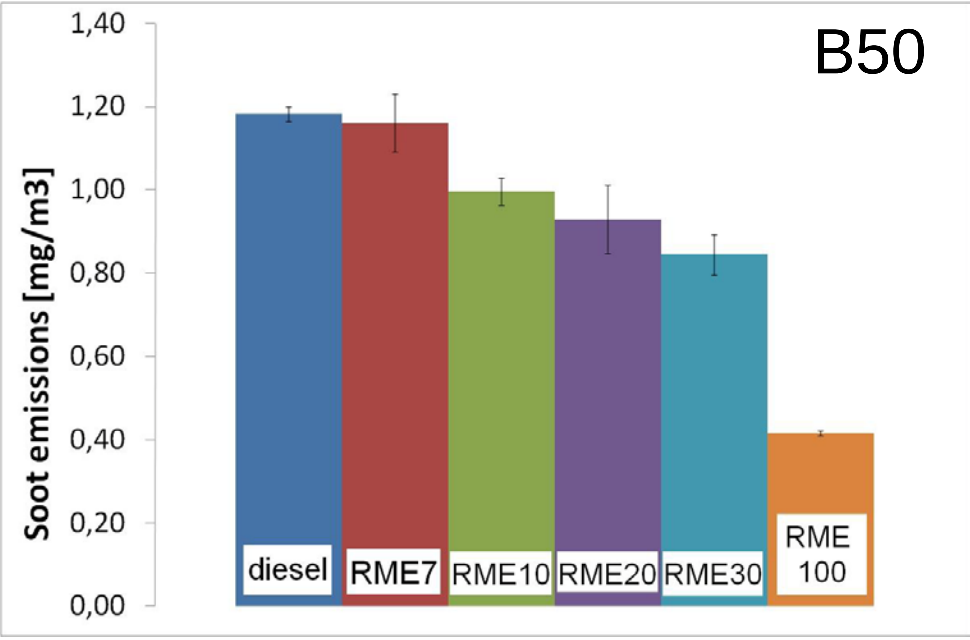
Soot & NO_x emissions

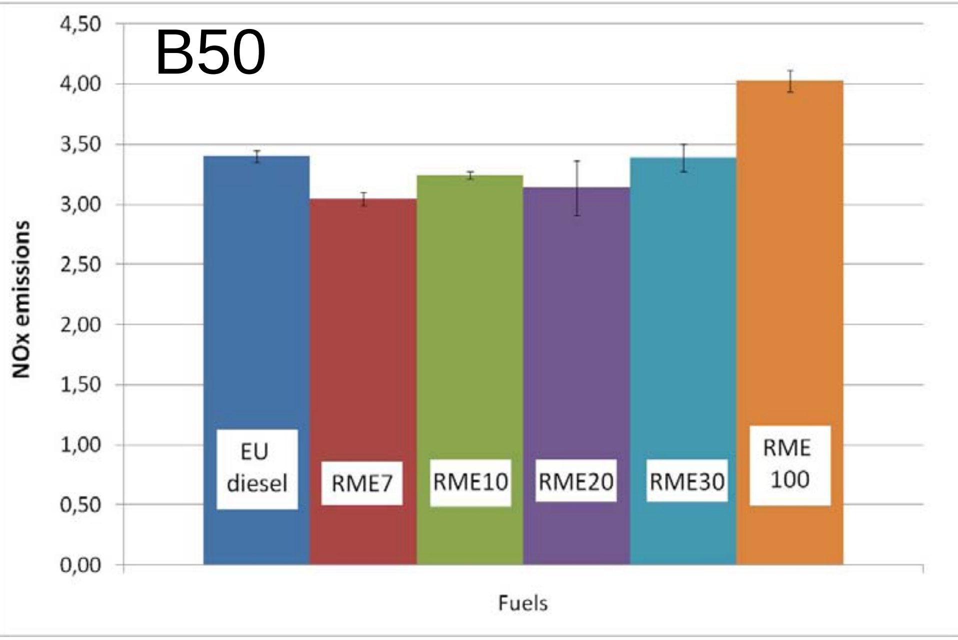
1,2 mg/m3 ~ 0,01 g/kWh (Euro VI)





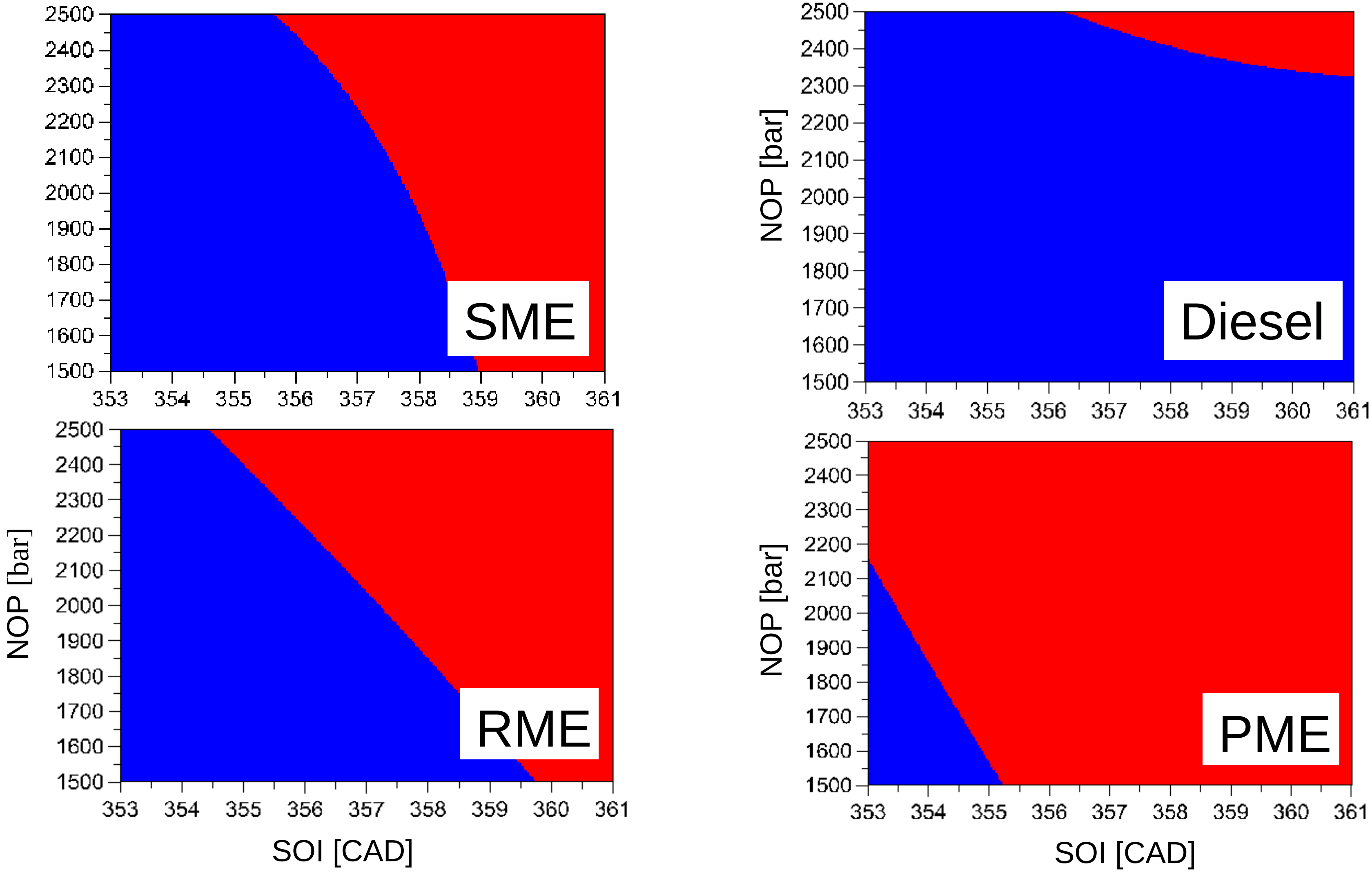
Soot & NO_x emissions, RME blends





Soot max 0,5 mg/m3 ~ 0,005 g/kWh
NOx 2 g/kWh

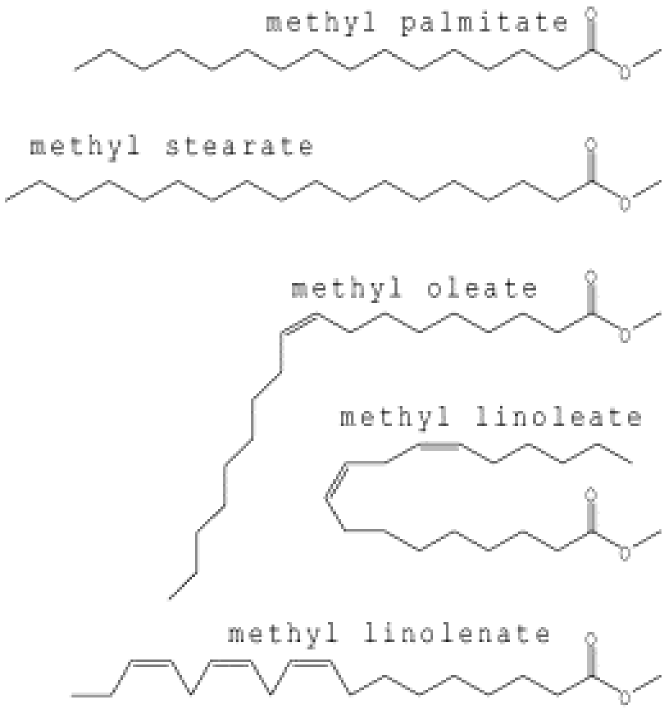
A25



Modeling:

Chemical Compositions of Bio-diesels

Esters	Formulas	RME	PME
methyl palmitate	$C_{17}H_{34}O_2$	4.2%	43.4%
methyl stearate	$C_{19}H_{38}O_2$	1.8%	4.3%
methyl oleate	$C_{19}H_{36}O_2$	61.1%	39.9%
methyl linoleate	$C_{19}H_{34}O_2$	20.0%	10.0%
methyl linolenate	$C_{19}H_{32}O_2$	9.4%	0.3%



Physical models

Rapeseed methyl ester (methyl oleate, $C_{19}H_{36}O_2$)

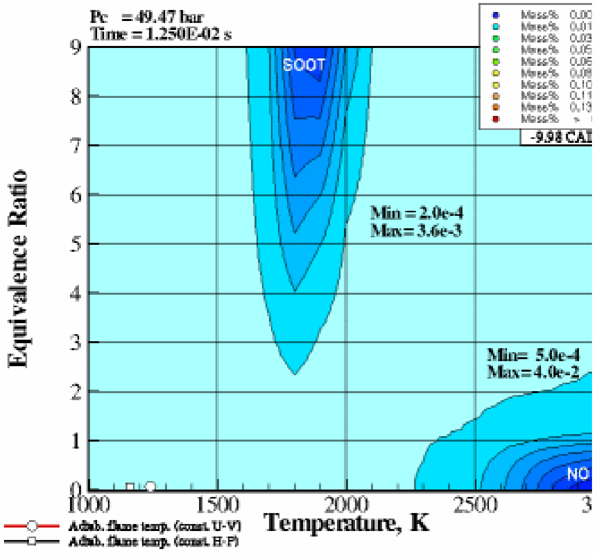
Diesel oil surrogate (conventional diesel oil)

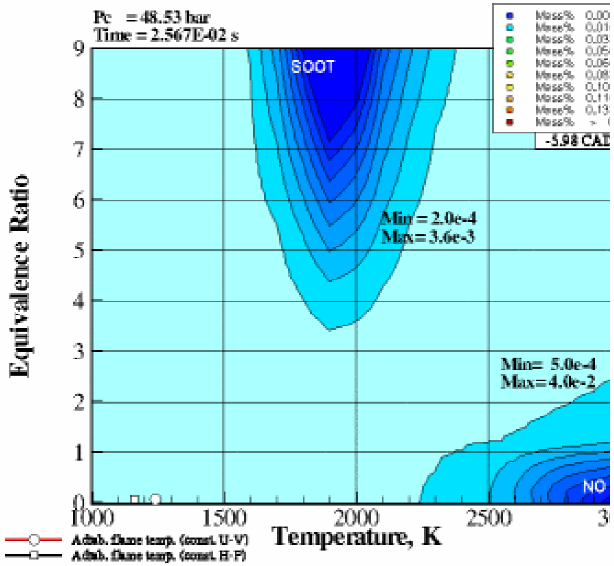
Chemical composition

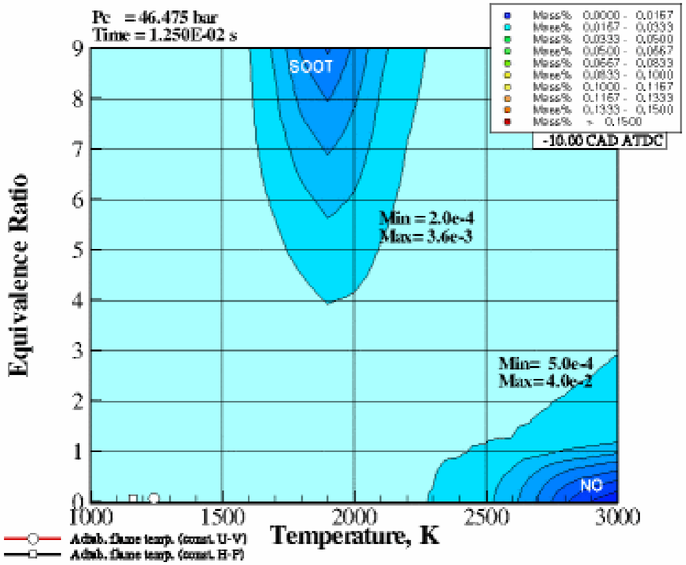
Physical model	Component	Formula
Rapeseed methyl ester (methyl oleate, $C_{19}H_{36}O_2$) →	Methyl butanoate	C5H10O2
	Methyl decanoate	C11H22O2
	Methyl propanoate	C11H22O2
	n-heptane	n-C7H16
	Allene	C3H4
Diesel oil surrogate (conventional diesel oil) →	n-heptane	n-C7H16
	Toluene	C7H8

Model description for RME50: DOS/RME 50:50%

Dynamic ϕ-T Parametric Maps



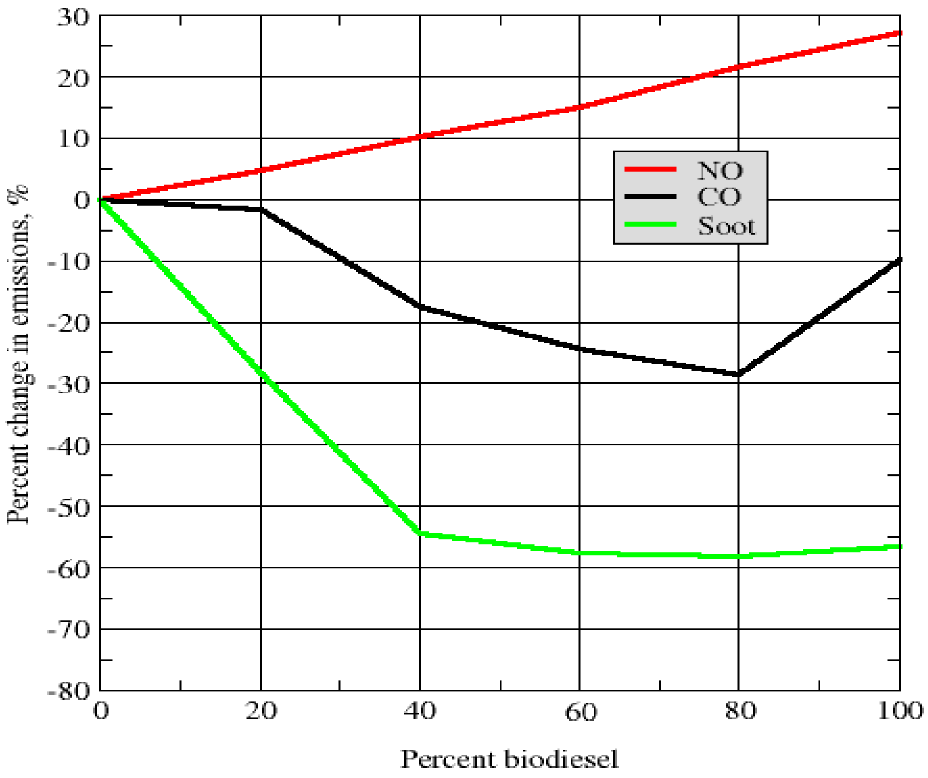




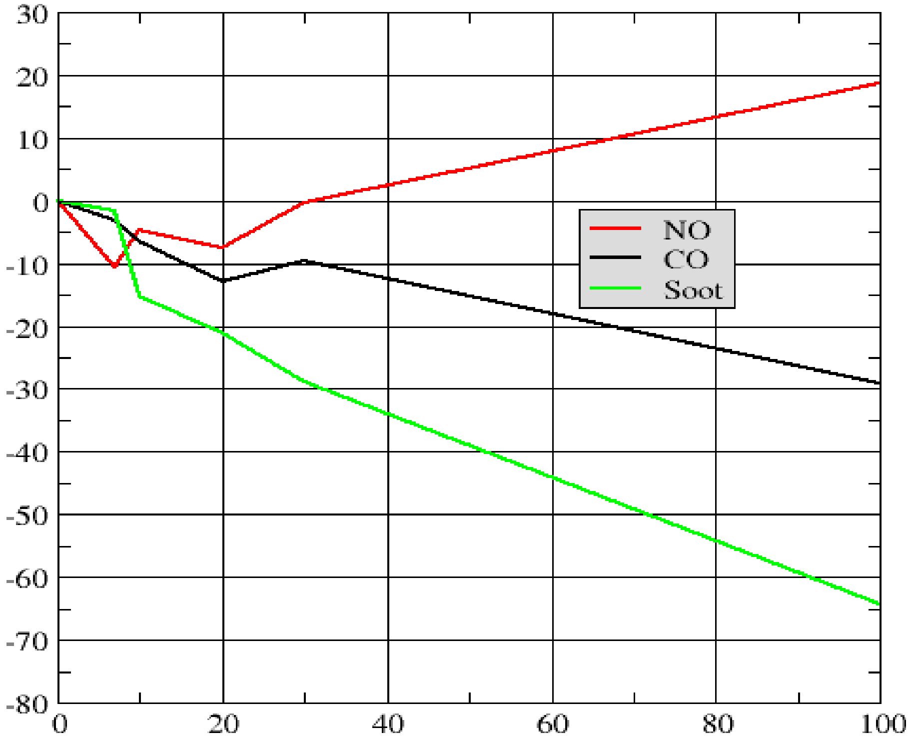
Diesel oil combustion RME combustion PME combustion

Comparison Experiments-Modeling

Emission Trends, Volvo D12C fueled with DOS/RME blends



modeling results



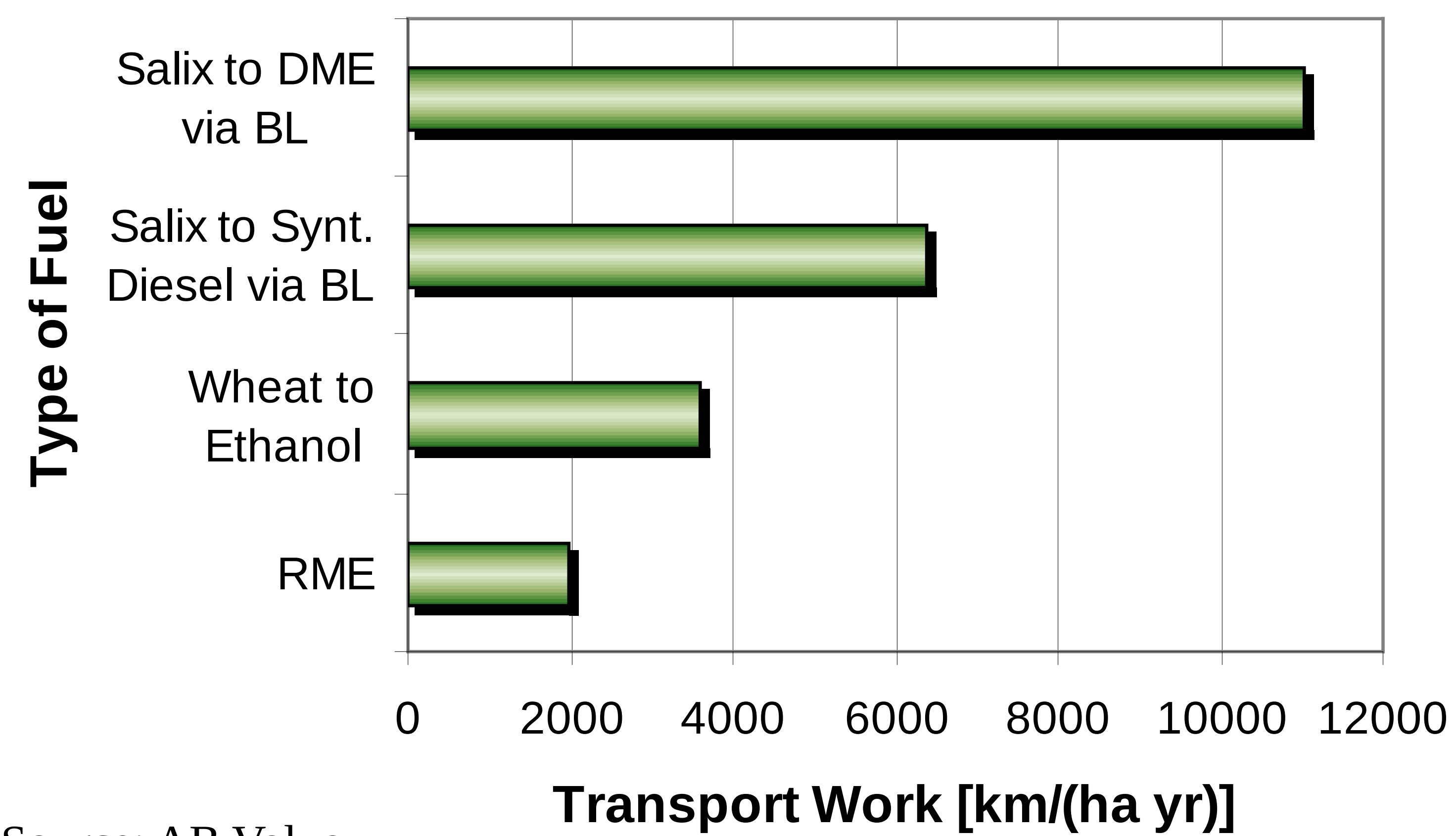
experimental results

DME

Henrik Salsing, Valeri Golovitchev and Ingemar Denbratt

Why DME as an alternative fuel?

- High life cycle efficiency

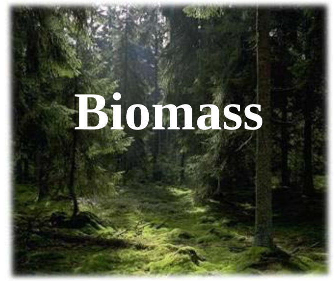


Source: AB Volvo

Why DME as an alternative fuel?

- Versatile

Feedstock



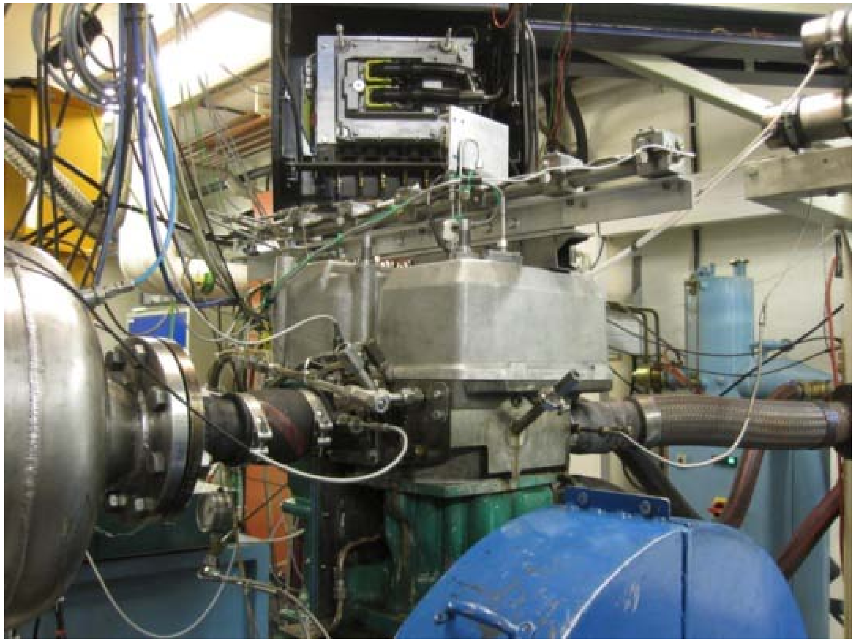
Production Process

End User

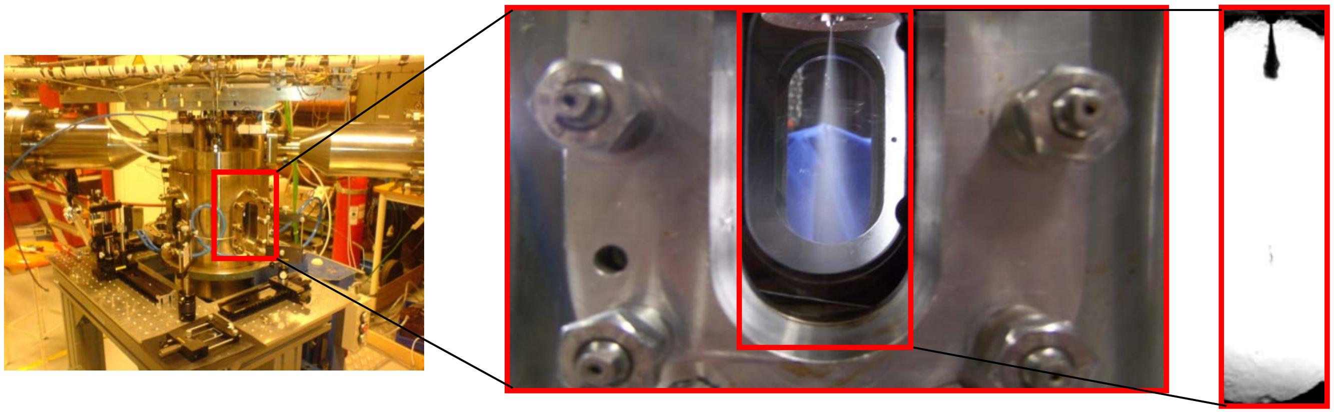
Experiments, engine

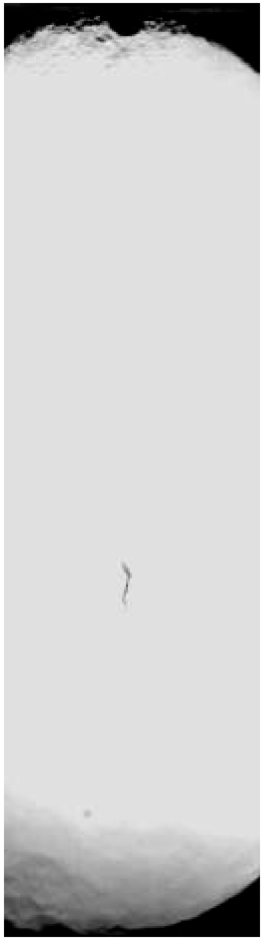
- Volvo D12 C single cylinder heavy duty engine
- Bore x stroke 131 x 150 mm
- Displaced volume 2.02 L

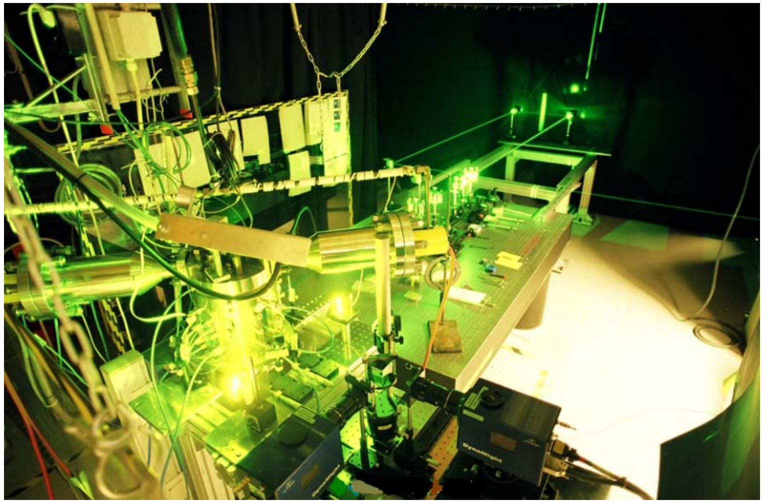
- Common rail system
- Rail pressure >300 bar
- Injector high flow design >2-3 times a standard injector

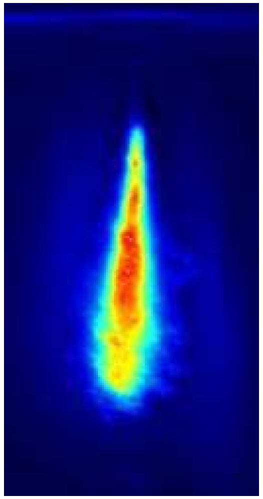


Experiments - Spray Chamber



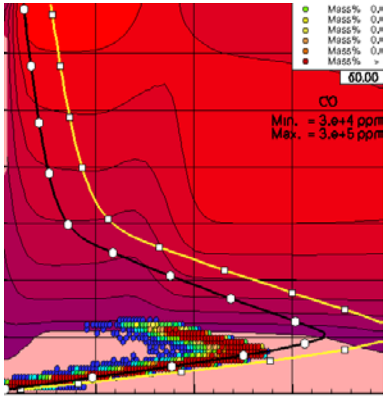


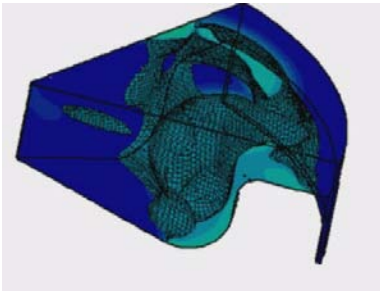


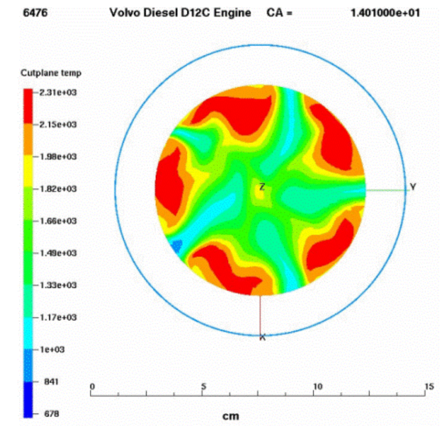


Modeling

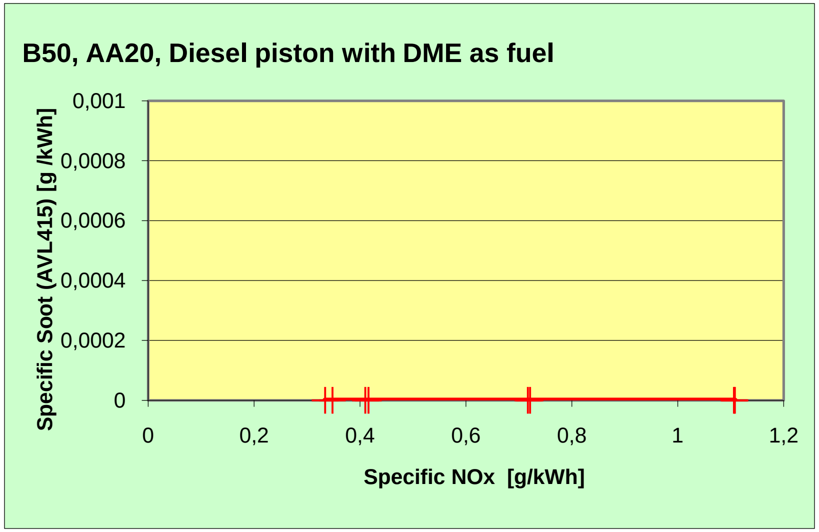
- Modeling of DME combustion based on detailed chemical kinetics in order to investigate, understand and suggest design of
  - Pistons
  - Nozzles





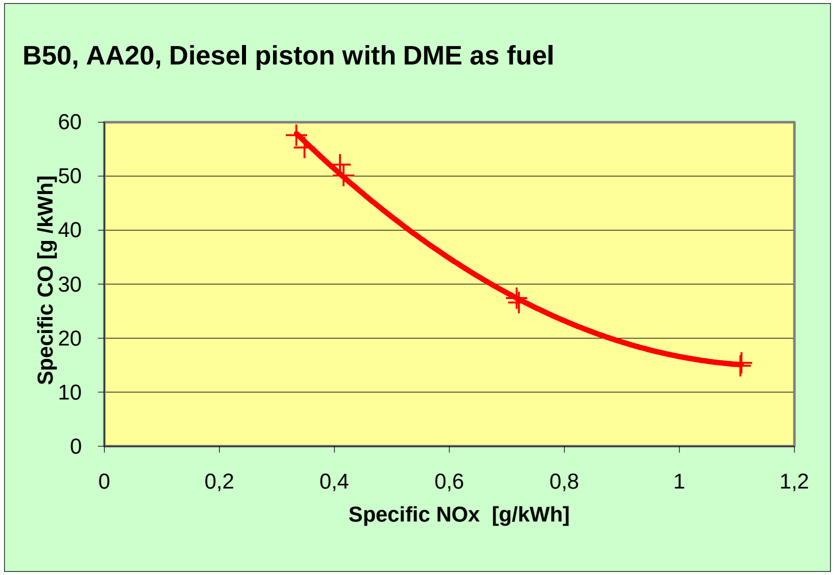


Results
-Soot, NO_x and CO

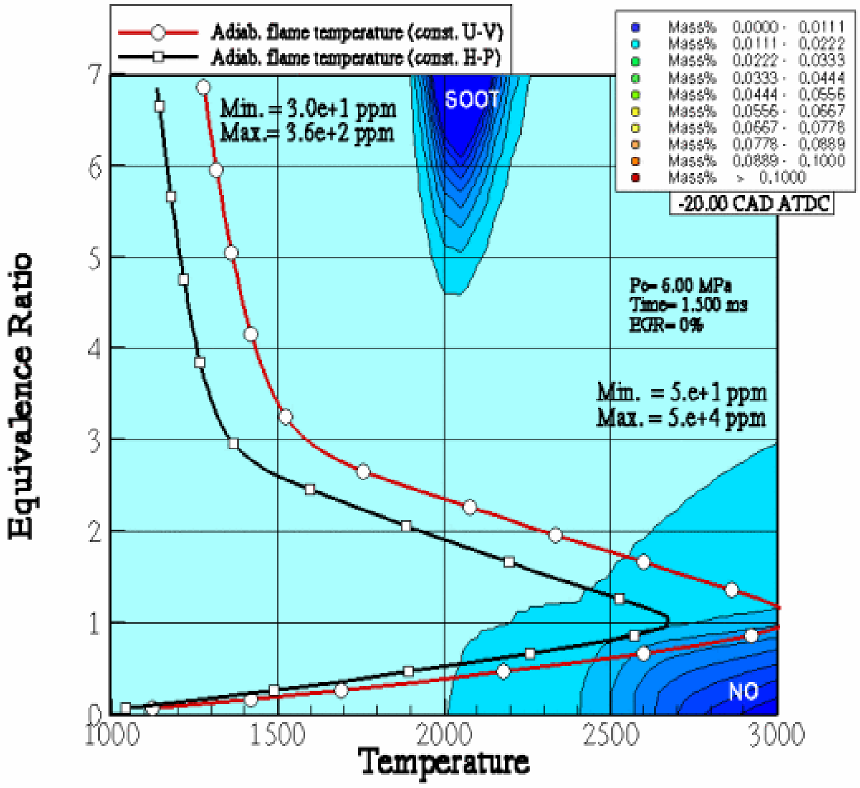


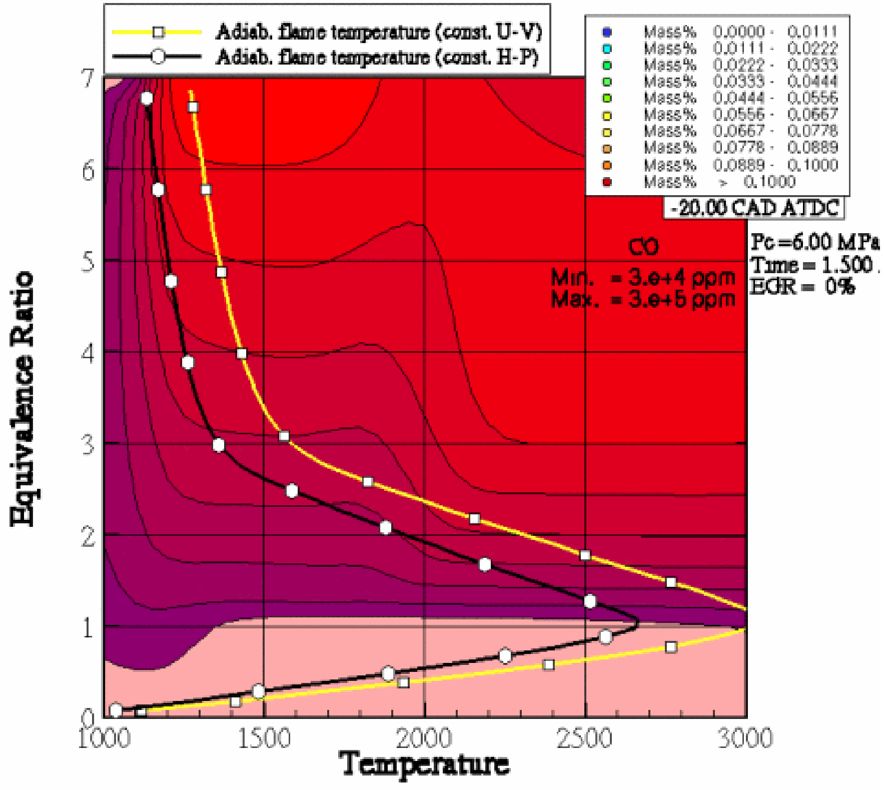
- Not relevant measuring soot with a smoke meter (AVL415 *e.g.*)
- More sophisticated instruments must be used (μ-soot, DMPS *e.g.*)

- At low NO_x conditions CO is the major emission from a DME fuelled engine



Results
-Soot and NO_x



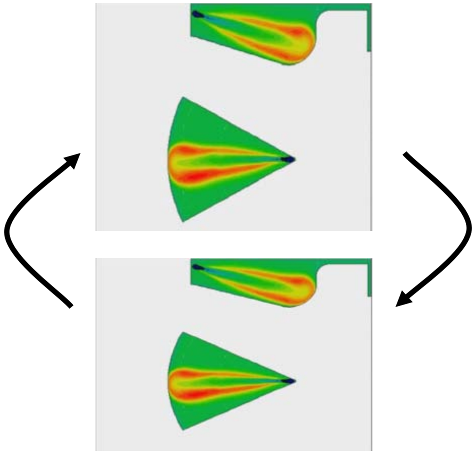


Results
-Piston shape

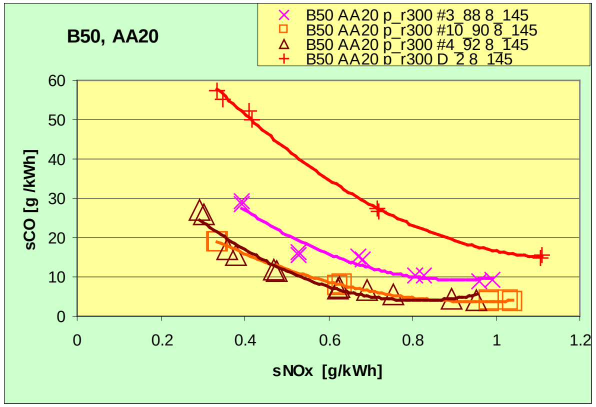
Simulations in combination with design of experiments

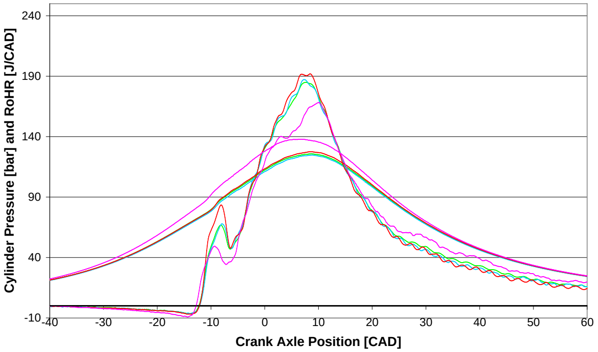
-Find parameters of importance

-Model the influence of the parameters



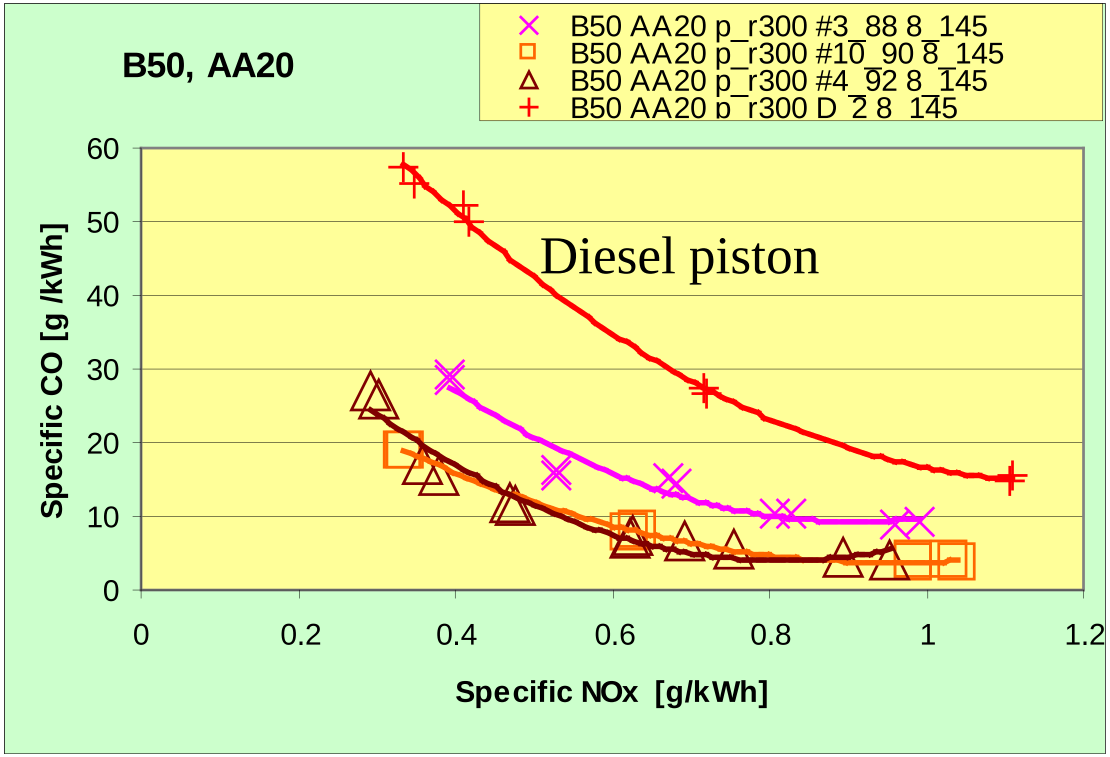
Experimental investigation





Results

- Influence of piston shape, CO – NO_x



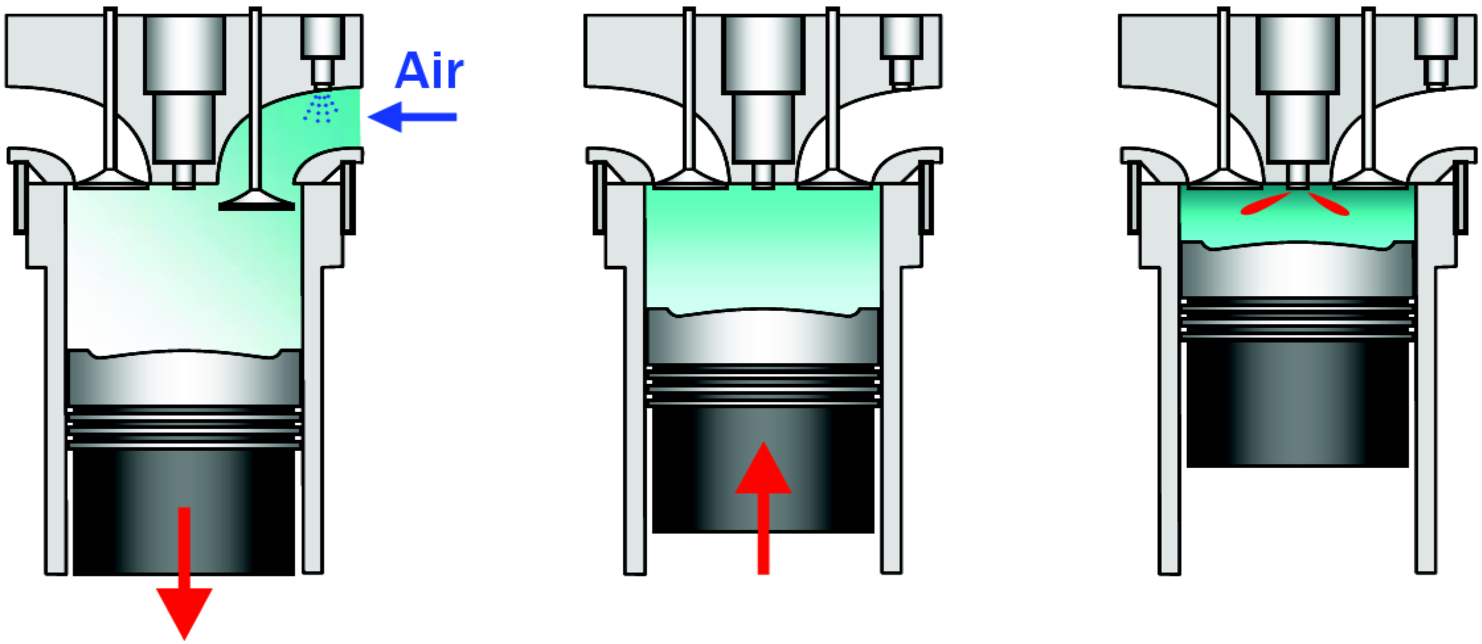
- A DME adapted piston result in significantly lower CO at the same NO_x-level

Dual Fuel

Valeri Golovitchev

Modeling of Dual Fuel, D-F, Combustion

Operational principle of D-F Diesel engine



a) Air intake and natural gas injection

b) Compression of air/natural gas mixture

c) Pilot diesel oil injection/ignition

Courtesy of: Yutaka Murata

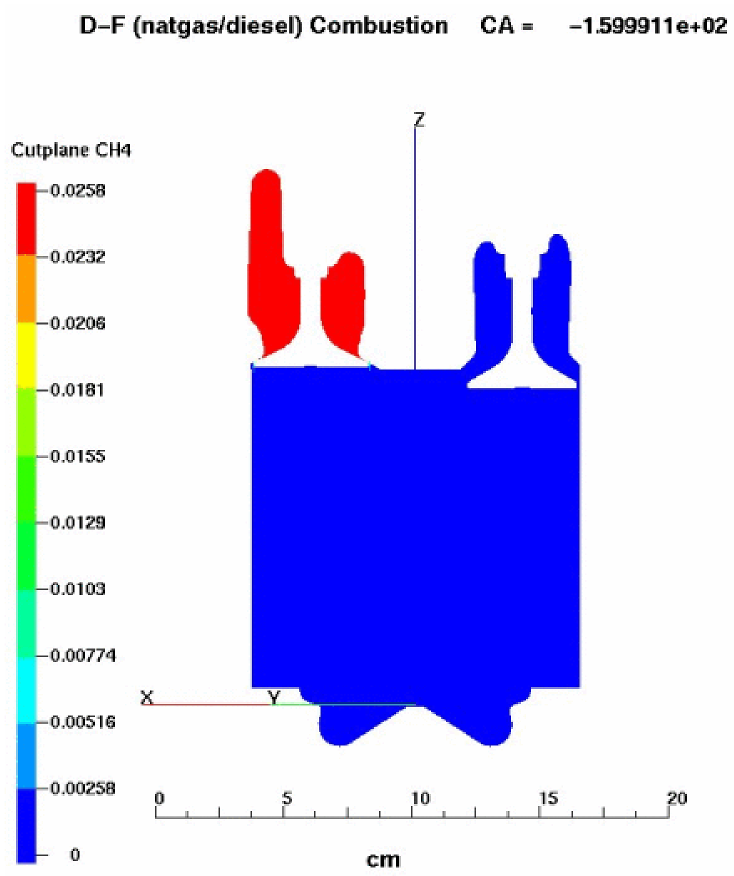
Modeling of Dual Fuel, D-F, Combustion

Computational models

Turbulence model	RNG k-ε model
Atomization model	KH-RT model
Collision model	Droplet trajectories
Diesel combustion	PaSR /DOS+nat gas
Flame propagation	TFC/Premix, Chemkin-2
NO_x formation	Extended Zeldovich
Combustion model	Coupled DOS/nat gas

Natural gas is considered as a blend of 87.8% CH_4, 5.9% C_2H_6, 4.6% C_3H_8, 1.7% C_4H_{10}
Chemical (coupled) mechanism: 76 species, 378 reactions

Preliminary results; Full cycle simulation



Summary FAME fuels:

- FAME fuels reduces soot emissions but increases NO_x
- FAME fuels with a higher amount of saturated hydrocarbons (PME) shows a smaller increase in NO_x
- Low blends of RME in Diesel oil can give slightly lower NO_x emissions (not captured by the simulations)
- A relatively good agreement between simulations and experiments was found

Summary DME:

- DME is an alternative fuel with a large potential
- The first DME adapted combustion system has been developed but it still suffers from too high CO emissions
- Further research and development is needed to improve and optimize the performance of DME combustion systems

Summary D-F modeling:

- A model for dual-fuel combustion (pilot Diesel Oil/Natural Gas) was developed
- D-F combustion for operational conditions similar to a conventional Diesel engine was predicted with a similar efficiency.
- Late cycle premixed combustion is presently too slow

Acknowledgements

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Thank you for your attention