Effect of Oxygenated Fuels on Soot From Diesel Spray

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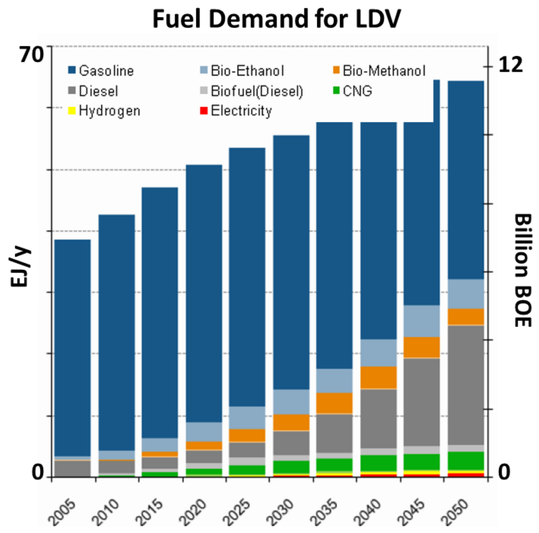
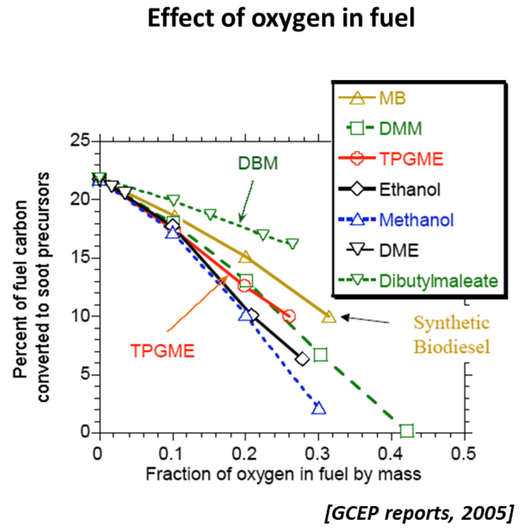
Motivation and Objectives



[WEC, Global transport scenarios 2050, 2012]



[GCEP reports, 2005]

- **Investigating the effect of oxygenated fuel properties on combustion and soot formation**
  - Simulations were performed to compare the oxygenated fuels and to give more insights between soot formation and an oxygenated fuel's molecular structure.

Methodology

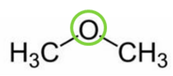
Fuel		O [#/mol]	C-C Bond [#/mol]	CN	MW [g/mol]	Ω_f * [%]	LHV [MJ/kg]
DME	CH_3OCH_3	1	0	55	46.1	14.3	28.9
TPGME	$CH_3OC_3H_6(OC_3H_6)_2OH$	4	6	63	206.3	12.9	28.1
MD	$C_{11}H_{22}O_2$	2	9	28	118.3	6.06	36.5
Hexadecane	$C_{16}H_{34}$	0	15	100	226.4	0	44.0
G60	TPGME:Hexa = 58:42**	2.3	9.8	-	214.7	6.06	35.1
M60	DME:Hexa = 84:16**	0.8	2.4	-	75.3	6.06	36.2

- **Fuel Oxygen Ratio** *[Mueller et al., 2003]*

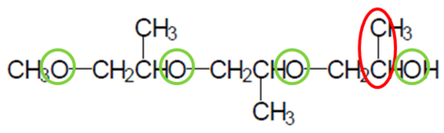
$$* \Omega_f = \frac{\sum_j a_j n_{O,j}}{\sum_m a_m \left(2n_{C,m} + \frac{1}{2} n_{H,m}\right)}$$

a : the number of moles
n : the number of atoms
j : fuel, k : oxidizer
m : fuel + oxidizer

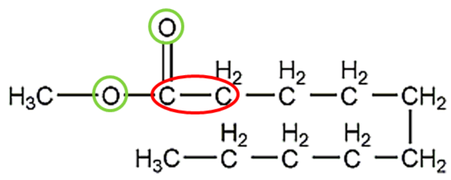
DME *dimethyl ether*



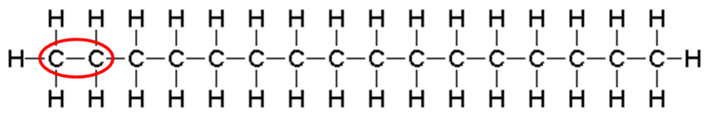
TPGME *tri-propylene glycol methyl ether*



MD *methyl decanoate*



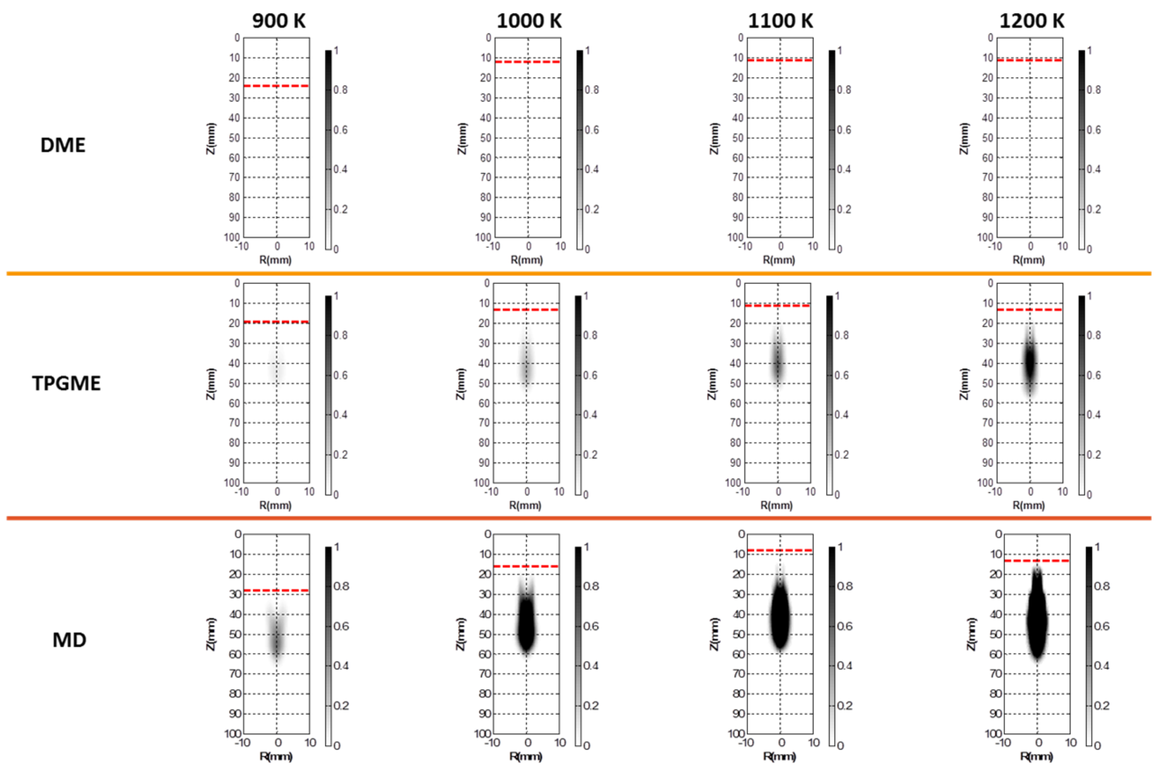
Hexadecane



- **Simulation Conditions: ECN 'Spray A' condition**
  - Ambient conditions : 22.8 kg/m3 / 800-1200 K / 15 % O2
  - Fuel mass / temperature : 18 mg / 363 K
  - Injection pressure : 150 MPa
  - 3D CFD code : KIVA-ERC with Chemkin
  - Fuel: TPGME [Park, 2014] , DME [Ra and Reitz, 2011], Hexadecane [Ra and Reitz 2015]
  - Soot model: multi-step soot model + PAH mechanism [Vishwanathan, 2011]

Results

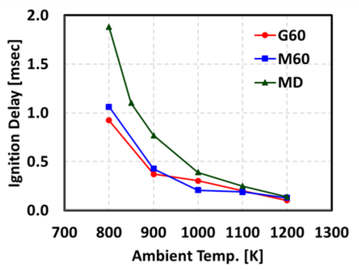
- **Effect of Fuel Molecular Structure on Soot**
  - The formation of soot decreases with increased oxygen content in the fuel and with decreased the number of C-C bonds. Fuel molecular structure strongly affects soot formation in addition to fuel-air mixing.

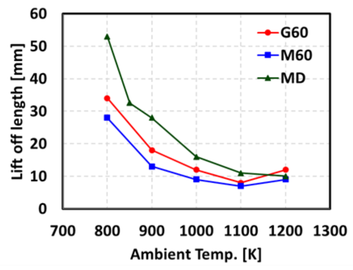


Fuel oxygen content ↑ → Soot precursor formation ↓

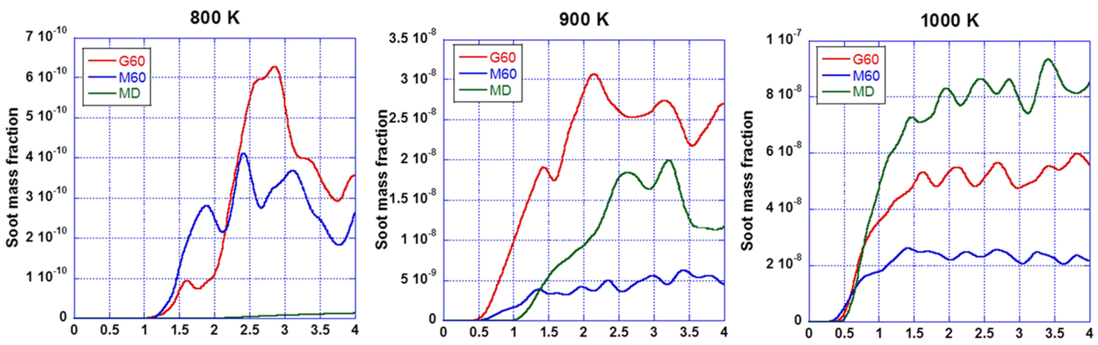
No. of C-C bond ↑ → Soot precursor formation ↑

- **Comparison of Fuel Blends**
  - The spray ignition delay and lift-off length control the soot formation for fuels with similar fuel oxygen ratio and the number of C-C bond.





Fuel	O [#/mol]	C-C Bond [#/mol]	Ω_f * [%]
MD	2	9	6.06
G60	2.3	9.8	6.06
M60	0.8	2.4	6.06



Summary

- **The effects of the oxygenated fuel properties on soot emissions were investigated.**
  - The formation of soot decreases with increased oxygen content in the fuel and with decreased the number of C-C bonds. Fuel molecular structure strongly affects soot formation in addition to fuel-air mixing.
  - The spray ignition delay and lift-off length control the soot formation for fuels with similar fuel oxygen ratio and the number of C-C bond.