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Performance Indicators for Biofuel Performances in Engine Applications

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Tailor-Made Fuels from Biomass –TMFB

- Lignocellulosic platform used to derive novel biofuels via selective production pathways.
- Prevention of competition with food production.

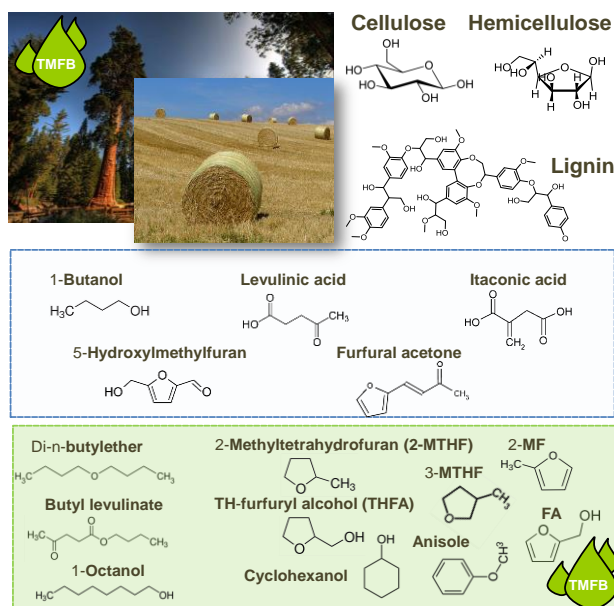


Figure 1. Biofuels production pathways from lignocellulose.

Biofuel combustion performance indicators

- Comprehensive study of the role played by the fuel on in-engine behavior.

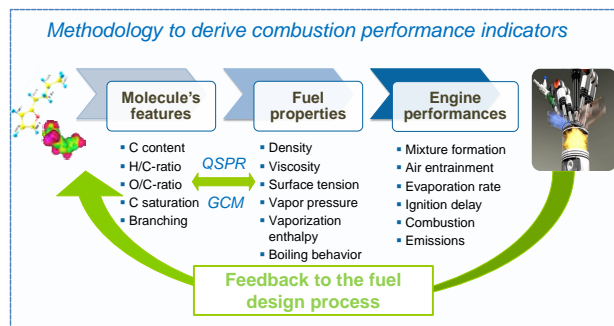


Figure 2. Research methodology for biofuels combustion indicators.

Fuel thermo-physical properties

Fuel thermo-physical properties predicted by a method based on quantum mechanics and the PC-SAFT equation of state [1].

- Prediction model coupled with one experiment allows increasing the accuracy of the property estimation.
- Accuracy of property estimation is improved from 14.5% (0 experiments) to 1.8% (1 experiment).

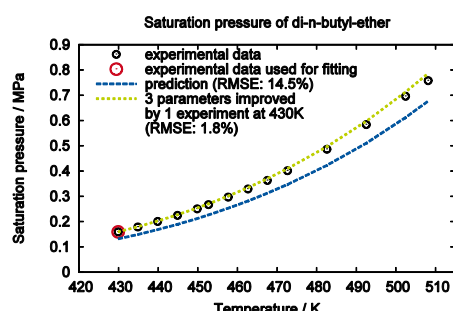


Figure 3. Improvement of three predicted parameters by a single experiment for Di-n-butyl Ether.

Material compatibility

Effect on engine related materials and components investigated experimentally for several biofuel candidates.

- Compatibility with elastomeric seals strongly depends on the combination of selected material and sealed fluid.
- 2-MTHF featured unacceptable property changes in all of the screened reference materials except for PTFE.
- Seal material needs to be selected individually.

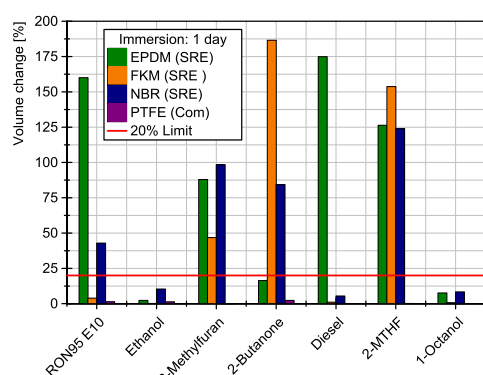


Figure 4. Swelling of NBR with representative fuel candidates.

References:

- Van Nhu N., Singh M., Leonhard K., *J. Phys. Chem. B* 112 (2008) 5693-5701. doi: 10.1021/jp7105742.
- Graziano B., Mora Perez J., Kremer F., Pischinger S., Heufer K. A., Rohs H., Proceedings of THIESEL conference, Valencia 2014.
- Graziano B., Kremer F., Pischinger S., Heufer K. A., Rohs H. SAE technical paper 2015-01-0890, 2015.
- Sudholt A., Cai L., Heyne J., Haas F. M., Pitsch H., F. L. Dryer., *Proc. Combust. Inst.* 35 (2015) 2957-2965.

Mixture formation influence on soot

- Influence of the properties of C8-C16 n-alkanes, 1-alcohols and di-n-ethers on the mixture formation studied numerically [2].
- Relevant engine boundary conditions considered.

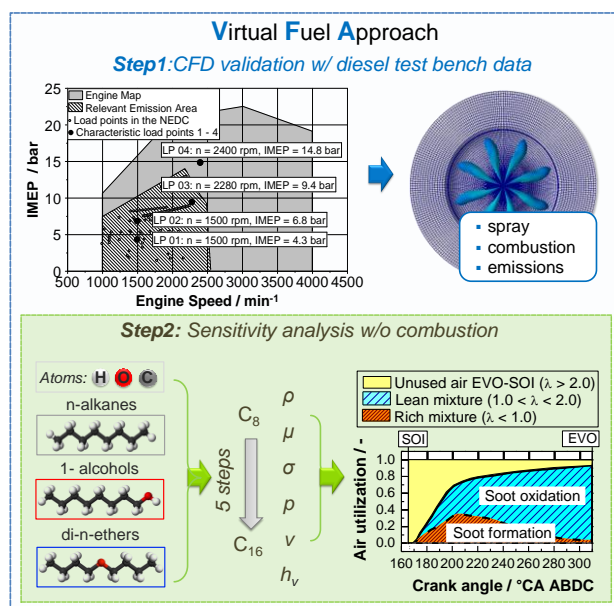


Figure 5. Main implementation steps of the Virtual Fuel Approach [2, 3].

Oxidation Potential Number

- A novel index to evaluate inherent soot reduction in D.I. diesel spray plumes is introduced.

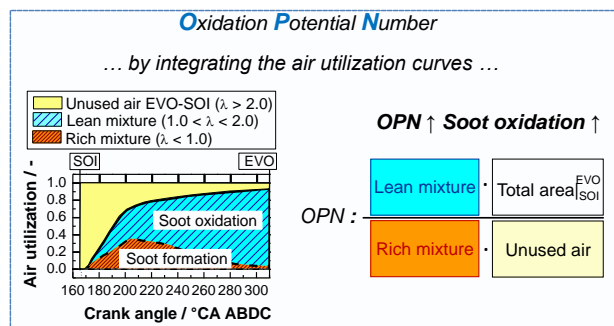


Figure 6. Introduction of the Oxidation Potential Number [3].

Inherent soot reduction behavior

- Fuel thermo-physical properties influence the mixture formation.
- Fuel thermo-physical properties' influence decreases as the engine operating load increases.
- Fuel impingement dominates over mixture formation process at 1500 rpm and 4.3 bar IMEP.
- C₈ molecules allow a more homogeneous air/fuel mixture, showing the highest OPNs.
- Among C₈ fuels, di-n-butyl ether features generally the highest soot reduction potential.
- 1-Alcohols feature overall lower OPNs.

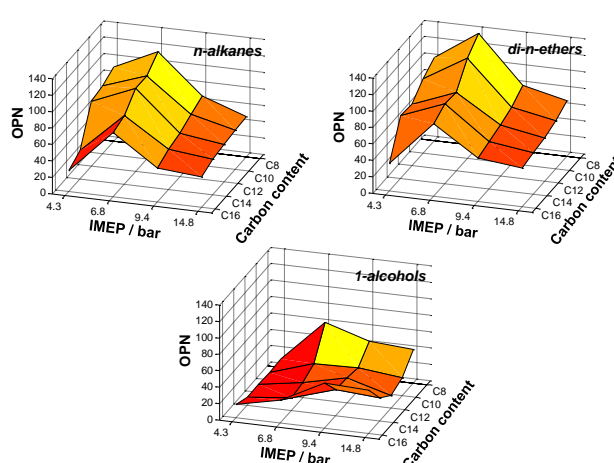


Figure 7. 3D-maps of OPN at varying engine operating conditions for C₈-C₁₆ n-alkanes, di-n-ethers, and 1-alcohols [3].

Auto-ignition behavior

Side chain and ring structure influences on Derived Cetane Number (DCN) investigated experimentally [4].

- H-abstraction at the carbon atom in the side chain adjacent to the ring for alkylated furans and at the carbon atoms adjacent to the oxygen in the ring for alkylated THFs.
- Side chain influence more distinct for THFs.
- Double bond influence dominates over side chain influence.

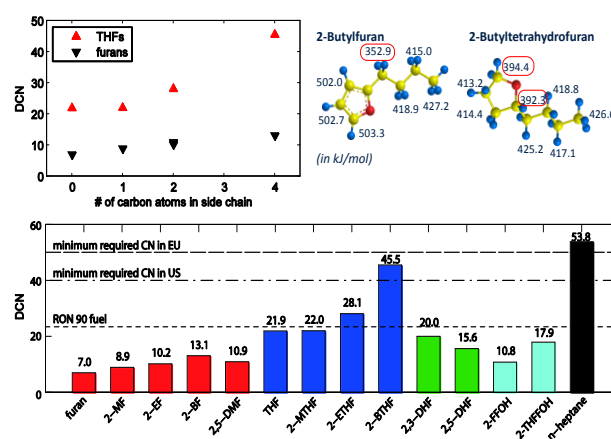


Figure 8. Side chain influence on DCN (top) and DCNs of alkylated furans, dihydrofurans and tetrahydrofurans (bottom).