JOINT FINAL EVENT

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Surrogate Composition, Mechanism Development and Reduction

Gasoline Surrogate Model Development

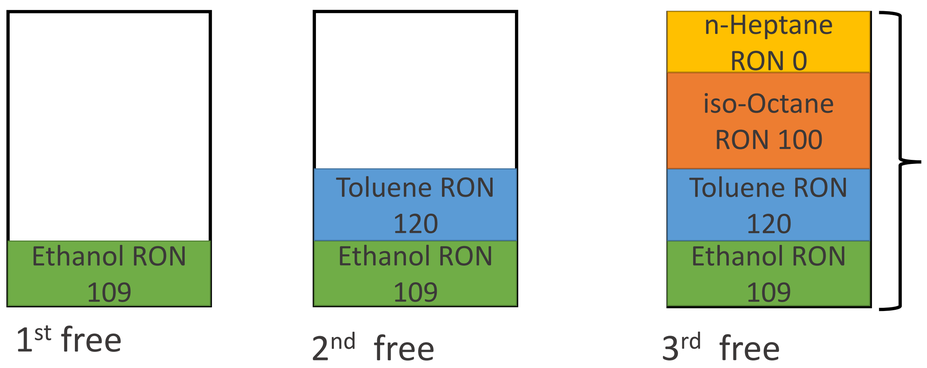
Surrogate combustion needs to capture:

- Combustion behaviour
- Physical properties of the liquid

Requirements on surrogate model:

- Reaction mechanism to predict gas phase combustion
- Emmission prediction (Soot, NOx, Hyrocarbons)
- Short CPU times

Ethanol Toluene Reference Fuel formulation

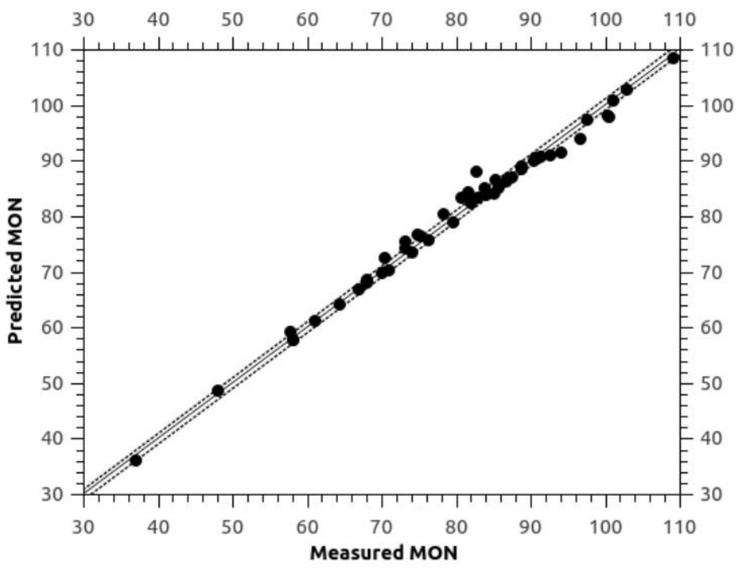


Calculate properties of the surrogate: Density, LHV, C/H/O ratio, Octane rating

1st free component: ethanol fraction taken from gasoline composition

2nd free component: Toluene fraction -> represents aromatic content in gasoline

3rd free component: RON of the gasoline -> calculate n-heptane and iso-octane fraction to match RON [11]

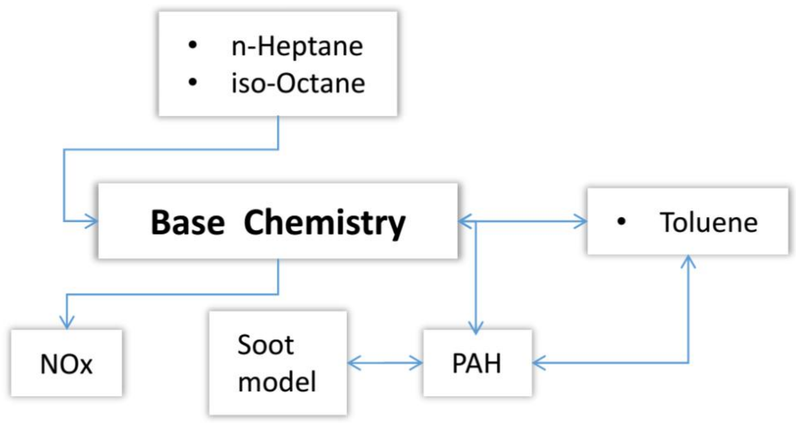


Plot to the left compares the measured motor octane number (MON) of different Toluene, n-Heptane, iso-Octane mixtures against the predicted MON using the procedure above with 0% Ethanol.

Conclusion

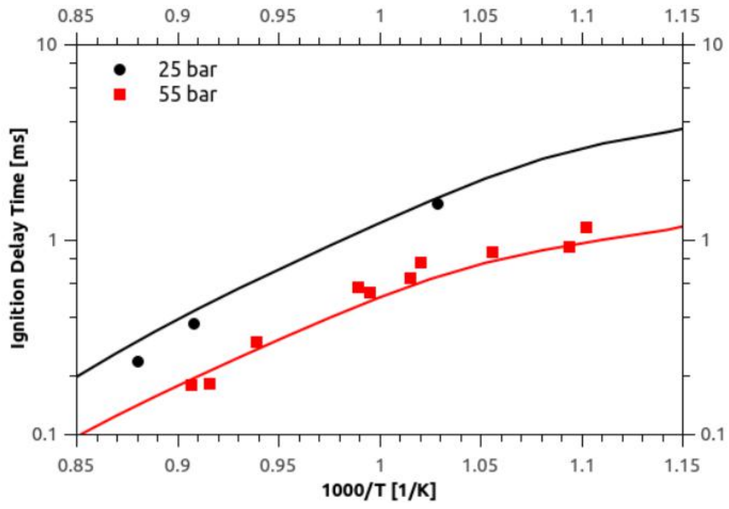
A complete tool chain for modelling gasoline combustion using a 4 component surrogate was developed. This enables for efficient and accurate combustion modelling including the prediction of auto-ignition as well as NOx and soot formation.

Variable Mechanism Concept



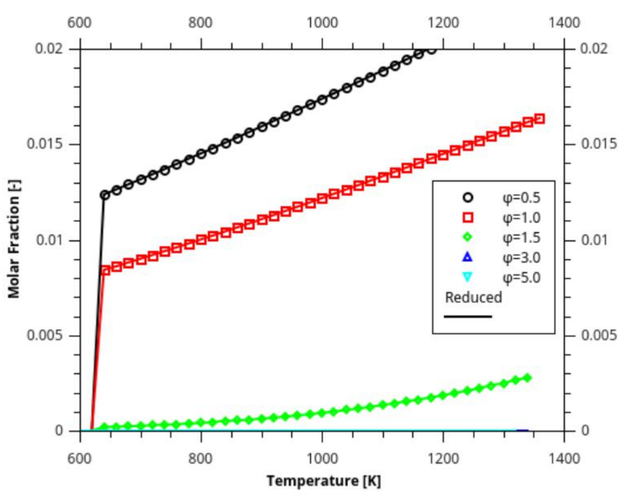
Base chemistry: C_1 to C_6 chemistry based on [1 - 5]
NOx chemistry: modified model based Lamoureux et al. [6]
n-Heptane model: modified model based on Seidel et al. [7]
PAH model: based on Moshammer et al. [8]
Detailed mechanism size: 476 species / 5160 reactions

Ignition delay time for surrogate of: 0.63 iso-octane, 0.20 toluene and 0.17 n-heptane (mole frac.) with artificial air at φ=1.0. Symbols Experimental data from Gauthier [9]; Line Model prediction



Mechanism reduction

The detailed mechanism was reduced by lumping similar species and than removing uncessary species as described by Seidel et al. [10]. The mechanism was reduced to 198 species and shows a good agreement with the detailed mechanism for the predicted major emissions, auto-ignition, as well as NO_x and soot formation. The reduction resulted in a speedup of factor 12.



Plot to the left shows a comparison of the predicted NO molar fraction of the gasoline surrogate fuel / air mixtures at different initial pressures, fuel equivalence ratios and temperatures. The solid line represent the reaction mechanism with 198 species and 1124 reactions; symbols detailed.

References: [1] Oßwald, P. et al. 2011, ZPCH (255) [2] Schenk, M. et al. 2013, Comb. & Flame (160) [3] Seidel,L. et al. 2013, Molecules (18) [4] Goos, E. et al. 2013, Proc. Comb. Inst. (34) [5] Nawdial, A. et al. 2015, Proc. Comb. Inst (35) [6] Lamoureux, N. et al. 2016 Comb. & Flame (163) [7] Seidel, L. et al. 2015, Comb. & Flame (160) [8] Moshammer, K. et al. 2017, Proc. Comb. Inst (36) [9] Gauthier, B.M. et al. 2004, Comb. & Flame 139 [10] Seidel, L et al. 2017, J. Eng. Gas Turbines Power. 2017 [11] Morgan, N. et al. 2010, Comb. & Flame (157)

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