Numerical and Experimental Comparison of Bio-Fischer-Tropsch Fuel and Commercial Diesel Fuel for Euro 5 Diesel Engine

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Introduction

Development of numerical tools for quantitatively assessing biofuel combustion in Internal Combustion Engines and facilitating the identification of optimum operating parameters and emission strategy are challenges of engine combustion research. Biofuels obtained through e.g. a Fischer-Tropsch process (FT) are complex mixtures of wide ranges of high molecular weight hydrocarbons in the diesel and naphtha boiling range dominated by C_{10}-C_{18} hydrocarbons in n-alkane, iso-alkane, alkenes, aromatic and oxygenate classes. In this paper modeling of combustion in a rapid compression machine has been performed using model compounds from a given FT biofuel distribution as surrogate fuels. Furthermore, the detailed mechanism has been reduced by applying an automatic necessity analysis removing redundant species from the detailed model. The reduced mechanisms have been optimized and evaluated for various surrogate fuels such as mixtures of nC_xH_{2x}+2, C_xH_{2x+2}-2 and C_xH_{2x-1} for x=8, 10, 12, 14, all present in the real FT biofuel, against the full mechanism. The reduced FT-mechanism will be used together with an appropriate diesel mechanism to study optimum engine performance and emission levels when using such fuels either in pure form or as blends in commercial diesel fuels as is common regulated by the EN standards for FAME type biofuels. This will be validated against experimental data carried out in a 1600 CC Euro diesel engine.

Development of reduced surrogate fuel mechanism for FT-biofuel

The FT biofuel from the biomass gasification reactor in Güssing[1] has been chosen as a reference fuel for the present study, and its composition is reproduced in Table 1.

Table 1: Hydrocarbon present in FT biofuel from biomass (approx. weight fractions)

	C10	C11	C12	C13	C14	C15	C16	C17	C18	C19	C20
n-Alkanes	13.21	6.79	8.46	9.87	10.51	9.49	8.14	5.26	2.82	1.28	0.51
i-Alkanes	0.13	0.45	0.51	0.64	0.64	0.45	0.26	-	-	-	-
Alkenes	1.60	3.72	3.72	3.33	2.44	1.67	1.67	0.38	0.13	-	-

Real FT biofuels are multi-component fuels and can contain up to dozens of different species. This is very difficult to incorporate in combustion modeling of such fuels, and no chemical model could be found that indeed accounted for oxidation paths for all the 26 species in the reference FT biofuel. However, a slightly reduced set of fuel species were chosen to represent the reference FT biofuel, based on available chemical models (denoted FT). The detailed mechanism from LLNL [2] was used as starting point for identification

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of a surrogate FT-fuel. Furthermore, in order to enable investigations of nitrogenous emissions (NOx) a sub-mechanism for nitrogen chemistry was implemented [3], resulting in a total of 7200 species. A slightly reduced set of fuel species were chosen to represent the reference FT biofuel (FT). Surrogate fuels varying chain length hydrocarbons such as C8, C10, C10-12, and C14 were used in RCM calculations in LOGEsoft [4] in order to investigate their applicability as surrogates for the reference. As shown in Figure 1 the surrogate containing C14 chain species performs well compared to the FT model fuel.

The detailed C14 mechanism was thereafter reduced in the RCM environment by employing necessity analysis and subsequently implemented into an advanced stochastic engine tool in LOGEsoft where injection, mixing, vaporization and combustion are modelled. Reduced mechanisms with increasing degree of reduction were tested. The optimum reduced mechanism contained a total of 1535 species (≈80% reduction).

The reduced FT-mechanism will be used together with an appropriate diesel mechanism to study optimum engine performance and emission levels, and validated against experimental data as given in Figure 2.

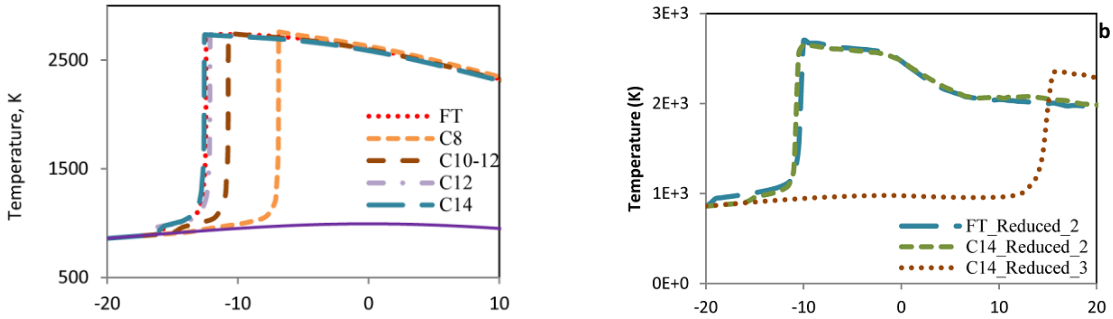

Figure 1: Temperature profiles for detailed FT- surrogate fuels (left) and reduced FT-surrogate fuels (right)

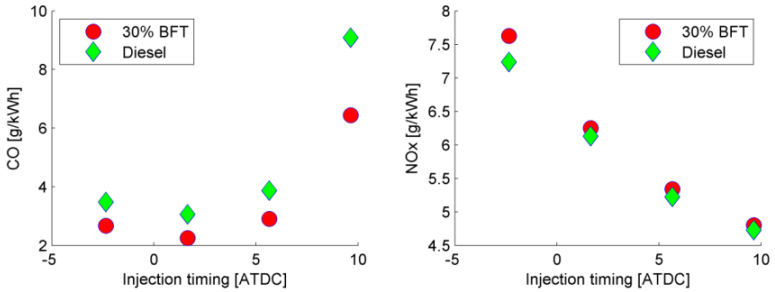

Figure 2: Emission levels measured at 40Nm and 1500 rpm with commercial diesel and a 30/70 blend with FT-biofuel [5].

References

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