

Comparative study of the high-pressure low-temperature oxidation of linear five-heavy-atom fuels: diethyl ether vs. *n*-pentane, and their mixture

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Abstract

We report for the first time detailed species profiles obtained at high pressure for the low-temperature (LT) oxidation of diethyl ether (DEE), a promising oxygenated bio-additive for dual-fuel compression-ignition engines. High-pressure effects on the DEE oxidation behavior were examined. DEE was then compared to its corresponding linear five-heavy-atom hydrocarbon fuel, *i.e.* *n*-pentane, to point out the influence of the fuel structure on their LT oxidation behavior. Finally, the oxidation of a mixture composed of these two fuels was investigated at different pressures up to 10 bar to investigate simultaneously the interaction of fuels and the effects of the pressure.

Experiments were performed using a setup of a high-pressure jet-stirred reactor (JSR) coupled to online gas chromatography (GC), with stoichiometric mixtures ($\phi=1$), residence time of 2 s, pressure range of 2-10 bar and temperature of 400-1100 K. About 20-30 species at each condition were detected. Based on our previous development, a combined LT kinetic model was updated with considering cross reactions between these two fuels. It was tested with these high-pressure data, showing a good predictive capacity, and subsequently assisting in the data interpretation.

Both experimental and modelling results show that: (i) Compared to 1 bar, high pressure does not significantly affect the starting reaction point of DEE (~425 K), but it strongly increases the global reactivity of this fuel and alters species formation. High pressure reduces both negative temperature coefficient (NTC) zones of DEE (classical and unclassical ones). This reduction results mainly from the change with pressure of competition between the thermal decomposition and the first/second O₂ addition of fuel radicals/hydroperoxyl-fuel radicals. (ii) Compared to *n*-pentane, DEE starts to react at much lower temperatures and it has a much weaker NTC as well as a significant difference in LT product distribution. Some analogous reaction classes, that are very important for the LT DEE oxidation, do not seem to be applicable for the case of *n*-pentane. (iii) DEE addition enhances strongly the reactivity of *n*-pentane in the fuel mixture. (iv) The reactor pressure significantly influences the reactivity of the fuel mixture in the range of 2.5-7 bar, however this influence becomes very weak when the pressure increases from 7 to 10 bar.