Experimental and modeling study of the pyrolysis and combustion of dimethoxymethane

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The urge to reduce the emission of greenhouse gases drives the blending of renewable fuels with conventional diesel. Oxymethylene ethers belong to a promising class of biomass-derived fuels which blended with diesel help to reduce particulate emission and to lower the carbon footprint. In this work, the combustion and pyrolysis of the simplest oxymethylene ether, *i.e.* dimethoxymethane, is studied experimentally and via first principles-based kinetic modeling. Experiments are performed in an isothermal jet-stirred quartz reactor (Herbinet and Battin-Leclerc 2014). Species mole fractions are measured at highly diluted conditions, four different equivalence ratios, *i.e.* $\phi=0.25$, $\phi=1.0$, $\phi=2.0$ and $\phi=\infty$, a temperature ranging from 500K to 1100K and a pressure of 1.07 bar. A total of 21 species are identified and quantified using three different online GC's. The main products detected during pyrolysis and oxidation experiments include CO, CO₂, methane, formaldehyde and methylformate. An increased reactivity at low temperature oxidation conditions is detected. A kinetic model is developed with the automatic kinetic model generation software tool Genesys (Van de Vijver et al. 2015). The primary decomposition and low temperature oxidation chemistry of dimethoxymethane is attained from quantum mechanical calculations at the CBS-QB3 level of theory. The model reproduces dimethoxymethane conversion and CO and CO₂ mole fractions well for all studied equivalence ratios as presented in Figure 1. The high yields of toxic formaldehyde raise the concern that oxymethylene ether blended diesel fuels may create emission problems.

Figure 1. Experimental (dots) and model simulated (lines) mole fractions for dimethoxymethane pyrolysis and oxidation. Mole fractions of dimethoxymethane (blue, full lines, ●), CO (green, dashed lines, ▲) and CO₂ (orange, dotted lines, ◆).

Herbinet, O., and F. Battin-Leclerc. 2014. International Journal of Chemical Kinetics 46 (10):619-639.

Van de Vijver, Ruben, et al. 2015. International Journal of Chemical Kinetics 47 (4):199-231.

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