Developing a predictive model for Novel Biofuel Molecules

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The world's increasing demand for transportation fuels – road, railway, air and sea – greatly depended on derivatives of fossil fuel. This heavy reliance coupled with the limited rate of fuel production has resulted in high fuel price volatility. Economical and environmentally friendly options are required to address this problem. Biofuels consists of methyl ester of fatty acids, usually derived from plant oils provide an alternative solution of shifting to low-carbon, non-petroleum fuels that play an important role in replacing fossil fuels in modern vehicles for the long run. Biofuels are not only beneficial for energy security; but it also reduces oil price volatility. It can also support economic development by creating new sources of income in rural areas.

Bisabolane contains branched chain cycloalkane. The implications of branching in alkanes on reaction mechanisms differ depending on the phenomena (e.g. laminar flame speeds, ignition delay times) as reported in several studies for mono-, di-, and tri-methylated alkanes. Because of its structural symmetry, and presence of branched alknaes, which are important components in conventional petroleum transportation fuels, present at a range of 40 – 60% in gasolin and approximately 40% in aviation fuel.[14] The degree of influence that alkane branching exerts on autoignition chemistry depends strongly on the temperature regime, which gives rise to distinct modes of chain-branching. Low-temperature chain-branching, occurring at temperatures below ca. 800 K, is driven by the addition of oxygen to alkyl radicals via $R + O_2 \rightarrow ROO$, subsequent $ROO \rightarrow QOOH$ isomerization, and second O_2-addition reactions thereafter proceeding to the formation of OH + a ketohydroperoxide that dissociates into two radicals. In the high-temperature regime, at temperatures exceeding 1000 K, the primary chain-branching mechanism shifts away from $R + O_2$-derived chemistry towards $H + O_2 \rightarrow OH + O$ and other small-molecule reactions. Ignition delay times are a critical modeling target in assessing such mechanisms given the importance of autoignition to the development of advanced, chemical kinetics-controlled combustion strategies. In contrast to the ignition behavior at high temperatures, differences approaching 10 ms were measured at temperatures below 800 K highlighting the role of the molecular structure of alkylperoxy radicals (ROO) on low-temperature chain-branching and autoignition. The difference correlates with the degree of methyl branching and the more rapid ignition for linear alkanes is due primarily to more facile $ROO \rightarrow QOOH$ pathways and subsequent ability for second O_2-addition via $QOOH + O_2$. In our group we will apply Component Centered (CC) approach and propose a surrogate biofuel molecule to study the complex biofuel molecules.