

Updating the Iso-octane Model

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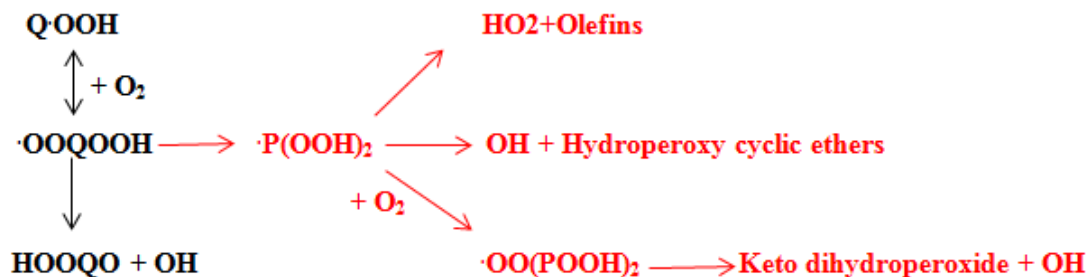
Abstract text

A better understanding of autoignition is crucial for modern compression ignition engines, especially homogeneous charge compression ignition engines (HCCI) which are driven by chemical kinetic processes [1]. A well validated mechanism enables accurate modeling of engines and better insight on the effect of fuel compositions on combustion phasing.[2]

Iso-octane is one of the main components in primary reference fuels (PRF), which are used as surrogates for simulating gasoline engine experiments. It is also considered as the 100 point on the octane number scale used for rating spark ignition fuels. Experimentally, iso-octane is either used as a neat fuel or in a fuel mixture.

In our work, we updated the iso-octane model developed by Curran et al.[3] with recently calculated rate parameters from literature . The new rates were calculated by various computational studies [4–7] using computational quantum chemical methods. In addition, new alternative pathways for peroxy alkylhydroxide ($\cdot\text{OOQOOH}$) were added.

The new model is validated against new rapid compression machine experiments (RCM) carried out at low temperatures [650 K-1000 K] for two equivalence ratios (1 and 0.4) and at pressures of 20 and 40 bar. Moreover, the new model was validated against shock tube data [8–11] and jet stirred reactor speciation data[12] from literature.



Conventional and alternative pathways for $\cdot\text{OOQOOH}$. The alternative pathway is shown in red

References

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