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The role of H_2O_2 at the onset of ignition of conventional and alternative fuels

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The decomposition of H_2O_2 ($H_2O_2(+M)\rightarrow OH+OH(+M)$) at low and intermediate temperatures is one of the branching mechanisms responsible for the ignition of hydrocarbon fuels [1]. H_2O_2 accumulates as a product of other reactions during chemical runaway, when the temperature is low. The accumulated H_2O_2 decomposes into OH radicals, which react with the fuel to produce water and heat, increasing the temperature until the chain branching mechanism driven by $H+O_2 \rightarrow O+OH$ takes over. H_2O_2 is also the characteristic feature of "knock" in spark ignition engines, and ignition in reacting systems like Rapid Compression Machines (RCM), Homogeneous Charge Compression Ignition (HCCI) and diesel engines. For fuels that exhibit two-stage ignition, the second stage is driven by the onset of H_2O_2 decomposition. Using tools of the Computational Singular Perturbation (CSP) algorithm [2,3], the substantial role of H_2O_2 decomposition was confirmed, as it was shown to be strongly related to the dynamics that drive the homogeneous autoignition of many fuels during the chemical runaway. As a result, a small fraction of H_2O_2 in the initial mixture decreases substantially the ignition delay time of fuel/air mixtures like methane, ammonia, methanol, n-butanol, ethanol and dimethyl ether (DME). The analysis was based on the identification of the characteristic time scale during the initiation of constant volume homogeneous autoignition and of the associated reactions and variables (species and temperature), by considering a wide range of values for the temperature, pressure and equivalence ratio.

References

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