Kinetics of the oxidation and autoignition of oxygenated fuels

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Recent challenges associated with the reduction of greenhouse gases and pollutant emissions have motivated interest in low temperature combustion engine technologies. In such engines, autoignition must be correctly timed for fuels that can exhibit negative temperature coefficient behavior. This can be challenging as in these low temperature conditions, the chemical kinetics responsible for oxidation and autoignition are extremely dependent on the fuel structure. It is therefore necessary to develop predictive models of the autoignition of engine-relevant fuels.

The recent interest for fuels derived from lignocellulosic resources has triggered experimental and modeling work on the combustion and ignition properties of furan and its substituted derivatives. However, their saturated counterparts have hardly been the subject of such interest, despite their interesting ignition behaviour, and frequent formation as intermediate products during the cool flame oxidation of hydrocarbons. This is a current modeling issue, as the concentration of these products is often not well reproduced correctly by the existing models.

Rapid Compression Machine studies provide a well controlled environment for such experimental studies, for pressures from 5 to 30 bar and temperatures from 600 to 1000 K relevant to these engine conditions. They are therefore suited to provide ignition delay data that constitute global model validation data. The RCM at University of Lille also provides the opportunity to extract samples of the reacting mixture during the ignition delay, providing in-

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sight into the composition of the unburned hydrocarbons formed in the cool flame, the main reaction pathways, but also detailed model validation data.

This experimental device is here used in order to describe the oxidation pathways of tetrahydrofuran and 2-methyltetrahydrofuran in engine relevant conditions.