A HIGH-REPETITION-RATE TIME-OF-FLIGHT MASS SPECTROMETRY STUDY OF 3-PENTANONE PYROLYSIS BEHIND REFLECTED SHOCK WAVES

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Amongst other ketones (e.g., acetone) 3-pentanone has gained importance as a fluorescence tracer in combustion studies. These tracers are used to monitor quantities such as temperature, fuel concentration or equivalence ratio under practically relevant conditions or in practical combustors, respectively, using non-intrusive laser imaging techniques [1]. Ketones are frequently used as tracers because their fluorescence can be excited by common UV lasers [1]. Despite the fact that 3-pentanone can be used as a tracer in combustion studies kinetic information such as rate constants or branching ratios is very scarce. Therefore, predicting the temperature-dependent decomposition as well as the interaction of the decomposition products with the fuel is difficult. Serinyel et al. [2] published a detailed oxidation mechanism for 3-pentanone, but still there is an urgent need for validated kinetics parameters such as decomposition rate constants. Therefore, we studied the thermal decomposition of 3-pentanone in the 1085–1400 K temperature range at pressures around 1.7 bar using a shock tube coupled to a high-repetition-rate time-of-flight mass spectrometer (TOF-MS) [3]. The investigated mixtures contained 0.5 or 1.0% 3-pentanone in neon. 1% argon was used as an internal standard for the mass spectrometer. The raw mass spectra were converted to absolute concentration-time profiles by calibration as described in [4]. Concentration-time profiles both for 3-pentanone and the main products (C_2H_4 and CO) will be presented and compared to preliminary results of simulations that are based on the mechanism given in [2].

References

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