ARAS-study kinetics oxidation of pentanol isomers behind shock waves

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In recent years, oxygenated fuels have taken on a prominent role as an alternative renewable energy source. Bioalcohols inhibit the formation of polyaromatic hydrocarbons (PAHs) and soot, and their additives improve the ignition and combustion efficiency of currently used fuels. However, a feature of the combustion of alcohols is the formation of harmful oxygen-containing by-products, such as aldehydes, nitrogen oxides NO_x, carbon oxides CO_x, etc., which makes it necessary to conduct detailed kinetic studies of the combustion chemistry of alcohol fuels. In this work, we studied the oxidation of n- and i-pentanol (n-$C_5H_{11}OH$, i-$C_5H_{11}OH$) at temperatures of 1600–3000 K and pressures of 2–3 bar. All experiments were carried out behind shock waves on a high vacuum kinetic shock tube in highly argon (Ar) diluted mixtures of 10 ppm fuel (n-$C_5H_{11}OH$, i-$C_5H_{11}OH$) with 10 ppm atomic/molecular oxygen (O/O_2). Quantitative measurements of the time profiles of the concentration of oxygen atoms in the ground electronic state $O(^3P)$ formed during the oxidation of pentanol isomers were first performed using the precise method of atomic resonance absorption spectroscopy (ARAS) in the vacuum UV region of the spectrum at the line of the oxygen atom at 130.5 nm. Along with experimental measurements, a detailed kinetic analysis of the oxidation of pentanol isomers was carried out according to modern kinetic schemes of biofuel combustion using the OpenSMOKE++ software package. The results obtained during a comprehensive study were successfully used to verify modern kinetic schemes for the combustion of promising biofuels in the studied temperature and pressure range.