

On the kinetics of oxidation of n-butane at high-pressure.

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Abstract

The autoxidation of n-butane was studied experimentally in a jet-stirred reactor at 10 atm over a range of temperatures (530-1030 K) and equivalence ratios (0.25, 1, and 1.5). Products of oxidation were analyzed in the gas phase by gas chromatography using several detectors (Flame ionization detector, thermal conductivity detector, quadrupole mass spectrometer), hydrogen peroxide analyzer, and Fourier transform infrared spectroscopy. Besides the n-butane and oxygen, 38 products were quantified. Kinetic modeling was performed using a kinetic reaction mechanism already used to simulate previous *n*-butane oxidation experiments in the cool-flame regime. Although improvements are needed to better describe the oxidation of *n*-butane under the present conditions, the model represents the major trends of n-butane oxidation. A kinetic analysis indicated the major reaction pathways to products and the sensitive reactions.