Kinetics analysis of phenol and benzene decomposition in supercritical water

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Abstract

Decomposition of phenol and benzene was studied in supercritical water (SCW) at 370–450 °C and 25 MPa over very short residence times (0.5–100 s). The study of simple model compounds such as phenol and benzene is an essential preliminary step to elucidate the primary mechanism of char and gas formation from lignin compounds. A quantitative detailed chemical kinetics model for the primary pathways of phenol and benzene decomposition in SCW was determined using the reaction pathways for its decomposition under supercritical conditions. The activation energy of benzene decomposition (91.16 kJ mol^{-1}) in SCW is much higher than that of phenol (54.17 kJ mol^{-1}) under similar experimental conditions. This emphasized the importance of the substituent group (hydroxyl group) in the benzene ring to enhance its decomposition rate. In addition, the reaction rate parameters, which are deduced for the overall reaction network of its decomposition under similar conditions, show good agreement with each another. Hence, the reaction rates of these reaction pathways are successfully described in this study.

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