239g Analyzing the Reaction Mechanisms at Supercritical Conditions through Bifurcation Theory

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Supercritical fluids due to their highly tunable properties with pressure and insignificant transfer resistances provide an attractive opportunity for reactions to be carried out at these conditions. Recently Supercritical water (SCW) oxidation process for treating organic waste is becoming a popular alternative for waste treatment and recovery. We describe an approach to analyze the reaction mechanisms at supercritical conditions through bifurcation theory. We developed the bifurcation diagrams in which pressure is selected as a bifurcation parameter and its effect on rate of reaction and solubilities of organic compounds in supercritical medium is analyzed. We also observed the multiplicities in reaction equilibrium constants and solubility. The information obtained through these bifurcation diagrams is utilized in explaining the complex reaction mechanisms at supercritical conditions. Through our approach we are describing the mechanistic behavior of SCW oxidation of different organic compounds like cyclohexane and tert-butanol.