413f Effects of Temperature, Pressure, and Oxygen Solubility in Liquid Phase Oxidation of Cyclohexane

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Cyclohexane oxidation in the liquid phase is of great industrial importance. Approximately 10^6 tons per year of cyclohexanone and cyclohexanol (also known as KA oil, Suresh et al., 2000) are made worldwide and used further in the production of adipic acid and capolactum, which are ultimately used in the manufacture of nylon-6 and nylon-6,6 (Schuchardt et. al., 1993). On the other hand, this process is one of the least efficient of all major industrial chemical processes as large scale reactors operate at low conversions. These inefficiencies as well as increasing environmental concerns have been the main driving forces for many studies and research (Suresh et. al., 2000). However, no systematic study on the effect of oxygen availability at different temperatures and pressures has been reported to date. Hence, there is still a lack of thorough understanding of hydrocarbon oxidation reaction mechanism and its effect on selectivity.

A new model of the process of liquid phase oxidation of cyclohexane, including reaction kinetics, mass transfer, and hydrodynamics parameters, is developed. The comprehensive kinetic model by Pohorecki et. al. (2001), multistage free radical chain reaction mechanism and kinetic rate constants determined by Kharkova et. al. (1989), and oxygen solubility in cyclohexane and values of Henry's constant from Suresh et. al. (1988) are used as a starting point. The influence of temperature, pressure, and oxygen availability on the reaction rate and the selectivity is determined. The new model enables the comparison of different types of reactors, namely, continuous stirred tank, bubble column, and microreactor. This study serves as a springboard to a deeper study of oxidation of hydrocarbons including the use of supercritical carbon dioxide and expanded solvents, which will increase oxygen solubility.

The project also aims of comparing modeling results with the experimental findings, in order to understand and determine the significance of most influencing parameters and examine the effect of various reactor designs.

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