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Diffusion and Chemical Reaction in Isobutylene Hydration Within Cation Exchange Resin

VIJAI P. GUPTA and W. J. M. DOUGLAS

McGill University, Montreal, Canada

The chemical reaction and diffusion rate parameters were determined for the hydration of liquid isobutylene to *t*-butanol with a cation exchange resin catalyst. High reaction rates were found to result from a high diffusivity of isobutylene within the resin catalyst. Both the high value for diffusivity and its negative temperature coefficient are consistent with the transport mechanism within the resin, being that of surface diffusion of isobutylene in an adsorbed state.

The hydration of isobutylene to *t*-butanol with cation exchange resin as catalyst is an alternative to the conventional hydration process, the hydrogen form ion exchange resin catalyst replacing the sulfuric acid normally used. The use of a resin catalyst gives rise to a three-phase system: an isobutylene-rich liquid phase, an aqueous liquid phase, and the solid catalyst. Phase equilibrium considerations indicate that one of the reactants, isobutylene, will be present only in very low concentrations in the hydrophilic resin phase. In spite of this the hydration rates are surprisingly high. Therefore the study was oriented toward obtaining an understanding of the mechanism of diffusion within the resin, since it appeared that this must be the key to the anomalously high reaction rates.

THEORETICAL MODEL

The theoretical model used contained the following assumptions.

1. Water is present in such large excess within the resin phase, relative to the isobutylene concentration, that the reaction should be independent of water concentra-

tion. Direct evidence for the validity of this assumption comes from the values of concentrations of isobutylene and water in the resin phase. The concentration of water in the resin was calculated from the data of Gregor et al. (1) and Pepper et al. (2). The concentration of isobutylene, measured as a part of this study (3), was found to be independent of butanol concentration over the existing concentration range. The equilibrium concentrations in fully swollen resin are:

Water	32.3 g.-moles/liter
Isobutylene	0.0172 g.-mole/liter

Furthermore, in the hydration of propylene with cation exchange resin catalyst, Kaiser et al. (4) also found the reaction rate to be independent of the concentration of water.

2. Reaction rate is first order with respect to isobutylene concentration. Lucas and Eberz (5) and Lashmet (6) have shown the reaction rates to be first order with respect to the olefin concentration.

3. Reaction is effectively irreversible for conditions of this study. The equilibrium constant for isobutylene hydration at 100°C. was determined by Smart et al. (7), who found, in terms of mole fractions, $K_x = 38$. For the range of reactant ratios used in this study, this equilibrium

Vijai P. Gupta is with E. I. du Pont de Nemours and Company, Inc., Wilmington, Delaware.