Determination of Kinetics Parameters for Gas-Phase Hydrolysis of AlCl$_3$

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In the present study, the kinetics of aluminum chloride (AlCl$_3$) hydrolysis was studied in a batch reactor (500 ml stirring tank). The degree of hydrolysis reaction rates were determined through concentration measurement of a product gas, HCl, by using Ion Chromatograph (DIONEX, ICS-150). The H$_2$O/AlCl$_3$ molar ratio were varied from 1.5 (stoichiometric ratio) to 15, the reaction temperature from 150 to 210°C, and the AlCl$_3$ concentration from 7.5×10^{-4} to 1.5×10^{-3} mol/L. The activation energy for early-stage hydrolysis were determined to be 88.1 KJ/mol from the experimental data and 72.2 KJ/mol by estimation using a molecular modeling program. The overall reaction rate was assumed to take the form as follow;

$$-r_{HCl}=(Ae^{-E/RT})C^{\alpha}_{AlCl3}C_{H2O}/1+k_2C_{H2O}$$

The temporal variation of the product gas (HCl) concentration was calculated using the kinetic parameters in the literature. The four parameter, A, E, α, k2 were determined to be 1.85×10^9 L$^{2.27}$/mol$^{2.27}$s, 35.8 KJ/mol, 2.27, 833.7 L/mol respectively, to that fit experimental data.