反应与分离

Preparation of Peracetic Acid from Acetic Acid and Hydrogen Peroxide: Experimentation and Modeling

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摘要　Based on the kinetic equations and equilibrium constants, some mathematic models were developed for calculating peracetic acid (PAA) concentration, equilibrium conversion rate of hydrogen peroxide, etc. The effects of several parameters on PAA synthesis were investigated by experimentation and modeling. The equilibrium constants determined from the forward and reverse rate constants at 293, 303, 313 and 323 K were 2.91, 2.81, 2.72 and 2.63, respectively. The models could predict the values of equilibrium concentration of PAA with average relative deviation of less than 10%. Both of the experimental and model-calculated results demonstrated that temperature and catalyst loading were the most important factors affecting the rate of PAA synthesis, but high temperature led to the decrease of equilibrium concentration of PAA. According to the model, the reaction could achieve equilibrium within 24 h when operated at 303 K with 1%~1.5%(w) sulfuric acid as catalyst. Additionally, when using anhydrous acetic acid and 30% hydrogen peroxide to prepare PAA, the volumetric ratio of the two solutions should be in the range of 1.2~1.5 in order to obtain the highest equilibrium concentration of PAA. This study can serve as a step towards the further optimization of PAA synthesis and some other related investigations.

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