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Kinetic modeling, thermodynamic studies and simulation of reactions with and without boiling using temperature-time information

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ABSTRACT

The measurement and modeling of the reaction kinetics for the hydrolysis and esterification reactions of acetic anhydride at temperatures up to 336K is discussed in this thesis. A new method for measuring the heat of reaction and the equilibrium constant for reversible exothermic reactions such as the esterification reactions of acetic acid and ethanol and acetic acid and propanol is proposed. Furthermore this thesis discusses the measurement, modeling and simulation of temperature profiles during the reaction of acetic anhydride and methanol, where reaction and boiling occur simultaneously. The experimental apparatus consists of an insulated, stirred batch reactor and a thermistor for measuring temperature. The temperature is measured as a function of time and the information is logged onto a computer for analysis and processing. The heat loss from the reactor was estimated by measuring the change in temperature with time during experiments where no reaction occurred. This data allowed us to estimate the overall heat transfer coefficient of the reactor and contents. The change in temperature as a function of time was logged during the experiments where reaction occurred. The heat loss for these experiments could then be estimated and the measured temperature profiles for the experiments with reaction could be corrected so as to be able to estimate the temperature versus time curves for an effectively adiabatic system. This allows us to relate the estimate adiabatic temperature to the extent of reaction. The hydrolysis reaction between water and acetic anhydride was first investigated under conditions of excess water and high temperatures between 300K -330K. The corrected adiabatic curves were used to determine the reaction kinetics and it was shown that at temperatures up to 366K the process still followed first order kinetics; this has not been reported previously in the literature. We also determined heat of reaction from the corrected adiabatic temperature-time curves and the average value that we obtained, 53.44 kJ/mol, was consistent with what is reported in the literature.However when experiments where performed on the same system but using excess acetic anhydride, the results showed a different behavior with kinetics suggesting a second order process.The heat of the reaction and the activation energy of this process was analyzed and found out to be 58.54kJ/mol and 37.10kJ/mol respectively. These results obtained from this excess acetic anhydride –water reaction which has not been studied in this manner before is surprising and is yet to be reported in the literature.

The reaction between acetic anhydride and methanol was studied between 290K and 300K and we found the process to be first order within this range of temperatures and heat of reaction of 61.58kJ/mol and activation energy of about 69.35kJ/mol respectively were obtained. The corrected adiabatic temperature profiles for the acetic anhydride- methanol reaction were used in modeling and simulation of temperature profiles in a batch reactive distillation system. The simulated temperature profiles in conjunction with thermodynamic considerations will be useful in the monitoring of concentration profiles in the reactive batch distillation systems.