

A STUDY OF KINETICS AND DYNAMICS OF
HYDROLYSIS OF ACETIC ANHYDRIDE IN BATCH AND
CONTINUOUS FLOW STIRRED TANK REACTORS

BY

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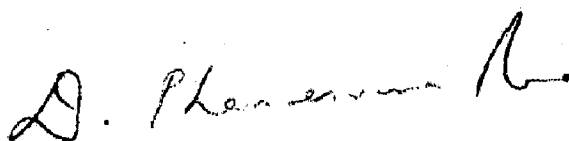
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CERTIFICATE

This is to certify that the thesis entitled "A STUDY OF KINETICS AND DYNAMICS OF HYDROLYSIS OF ACETIC ANHYDRIDE IN BATCH AND CONTINUOUS FLOW STIRRED TANK REACTORS" being submitted by Mr. Natesan Subramanian Jayakumar to the Indian Institute of Technology, Delhi, for the award of the degree of DOCTOR OF PHILOSOPHY is a record of the bonafide research work carried out by him. Mr. Natesan Subramanian Jayakumar worked under my guidance for the submission of this thesis which to my knowledge has reached the requisite standard.

The thesis or any part thereof has not been submitted to any university or Institute for the award of any degree or diploma.



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ABSTRACT

Mathematical modelling and experimental verification of the steady state and dynamic behaviour of a continuous flow stirred tank reactor is useful for designing a safely operable CSTR with suitable control. In the present work, hydrolysis reaction of acetic anhydride in the presence of acetic acid as solvent was chosen for experimental study of the dynamics of a CSTR.

The kinetics of hydrolysis of acetic anhydride in acetic acid was studied under isothermal conditions. Batch isothermal experiments for an initial concentration of acetic anhydride equal to around 7.0 gm. moles/litre were conducted at various temperatures between 20.5°C to 41°C. The reaction system was found to obey second order rate law and the values of the kinetic parameters, activation energy and frequency factor, obtained in this study were found to be equal to 15226 cal/(gm.mole) and 4.64×10^{10} cc/(gm.mole)(min) respectively.

In order to verify the validity of hydrolysis reaction of acetic anhydride in the presence of acetic acid at high temperatures and various concentration levels as well as understand modelling of nonadiabatic batch

reactor dynamics, experiments were conducted at an initial concentration of acetic anhydride equal to 5 gm.moles/litre and 2.5 gm.moles/litre in a batch reactor. Heat loss experiments were conducted by using the batch reactor for determining the values of natural convection heat loss coefficient and radiation heat loss coefficient. Values of rate constants and kinetic parameters were calculated from batch reactor data by employing two different estimation methods.

The values of second order frequency factor, and activation energy were found from non-adiabatic batch reactor studies to be equal to 34.89×10^{11} cc/gm.mole)(min) and 17948°K respectively. However, different values of kinetic parameters were obtained from different runs. The observed variation of the values of the kinetic parameters was assumed to be due to either the concentration levels of the reactants and solvent employed or the impurities present in the reactants and solvent Or due to all of them

CSTR experiments were conducted to verify the existence of multiple steady states by employing a feed concentration of acetic anhydride around 5 gm.moles/litre and residence times in the range 2.5 to 5 minutes. Three different sets of CSTR experiments were conducted corresponding to different values of mean residence time and feed concentration which proved the existence of steady

state multiplicity. Theoretical interpretations of the CSTR steady state and transient data were attempted with the help of mathematical models. Upper stable steady state temperatures, as well transients reaching upper stable steady state temperatures could not be predicted well, whereas lower stable steady state and transient data reaching lower stable steady states could be predicted reasonably well. The reason for the mismatch between theory and experiment in the case of runs reaching the upper stable steady state was thought to be mainly due to uncertainty in the values of kinetic parameters used in the model.

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