Scope and Objectives
SCOPE AND OBJECTIVES OF THE PRESENT WORK

Catalysis finds widespread applications in almost all the fields of chemistry and chemical engineering both in laboratories and in industries. The homogeneous catalysts are used in different reactions viz., hydrolysis of esters, esterification, chlorination, hydration, free radical polymerisation, isomerisation and alkylation etc. Heterogeneous catalysts are extremely important in a number of industrially important processes. Phase transfer catalysts (PTC) and polymer-supported (both organic and inorganic) phase transfer catalysts (Triphase catalysts - TPC) viz., polymer-supported ammonium and phosphonium ions, crown ethers, metal complexes etc. are also employed as catalysts to study a variety of reactions such as C-alkylation, hydroxylation, epoxidation, isomerisation, dichlororocarbene addition, O-alkylation etc.

Investigations carried out so far on the preparation and study of complexes of SnCl$_4$ and ZrCl$_4$ with pyridine and poly (vinylpyridine) as ligands deals with hydrogenation of aldehydes and alcohols, acetalisation and ketalisation, esterification, oxidation of alcohols, reduction of ketones and carbonyl compounds, aldol condensation etc. There is no report on the systematic kinetic study of the soluble Py-SnCl$_4$ and Py-ZrCl$_4$ and polymer-supported - SnCl$_4$ and polymer-supported - ZrCl$_4$ catalysts on the esterification of acetic acid with 1-hexanol, phenethyl alcohol and cyclohexanol.
In the present study, it was proposed to prepare the soluble Py-SnCl$_4$ and Py-ZrCl$_4$ and insoluble polymer-supported SnCl$_4$ and polymer-supported ZrCl$_4$ catalysts and characterise them using FT-IR, UV and elemental analysis. It was further proposed to study the kinetics and mechanism of the esterification reactions. To begin with, the esterification of acetic acid with 1-hexanol will be carried out to assess the efficacy of the catalysts. We propose to use the more efficient catalysts to study the kinetics of esterification of phenethyl alcohol and cyclohexanol.

To arrive at the kinetic results, it has been proposed to carry out the esterification by varying the fundamental physico-chemical parameters such as stirring speed, substrate concentration, catalyst amount, percent active site, percentage of crosslinking, particle size and temperature on the kinetics of the esterification reactions.

It was also intended to compare the activities of the insoluble and soluble catalysts under triphase and biphase conditions in the esterification reactions.

It was also proposed to evaluate the energy of activation (Ea) and other thermodynamic parameters (A, $\Delta H^\circ$, $\Delta S^\circ$ and $\Delta G^\circ$) for the above biphase and triphase reactions under identical conditions using these complexes which are not available in literature. Based on the results, suitable reaction mechanism(s) will be proposed.