

An Indian-Australian research partnership

Catalytic and reaction engineering studies on organic liquid phase oxidations

Project number: IMURA0083

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Research Academy theme/s

List only the research academy theme/s that is relevant to the project

1. Advanced computational engineering, simulation and manufacture

The research problem

As a class of reactions, organic oxidations account for a large proportion of industrial activity in various sectors such as petrochemicals, polymers, fine chemicals, etc. In a number of situations, the reaction uses air as the oxidant and the reaction is in the liquid phase. Mechanistically, many of these reactions can be studied as a class because of common features and similar intermediate reactions. There are problems of selectivity arising out of the complexity of the underlying reaction mechanism. Traditionally, the oxidations have been carried out either with homogeneous catalysts or in the absence of any catalyst. The catalytic principles that are useful have been identified and studied in considerable depth. Recently, there have been developments in catalysis due to advances in nanotechnology, and we propose to study some of these developments in the context of liquid phase organic oxidations. The selectivity issues can also be addressed in multifunctional reactors, which forms another prong of the study. It is possible to combine the two ideas, namely, of (heterogeneous) nanocatalysts and of multifunctional reactors, in a configuration such as Reactive distillation. The motivation for this research comes from recent findings of high activity and selectivity in alcohol oxidations, of a normally inert material such as gold. Preliminary considerations also indicate the potential benefits of reactive distillation towards improving the selectivity of several oxidations of industrial importance.

It is envisaged that the study would involve both experimentation and modelling. The experimental component would comprise of catalyst development, characterization, and kinetic studies, and modelling, in the areas of kinetics, reactor studies and nonlinear dynamics. The reactor studies and modelling will be carried out primarily in IITB and catalyst development and characterization, primarily at Monash.