IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Heterogeneous catalysis of cyclohexane oxidation**	
Project Number	**IMURA0677**	
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IITB Department:	Chemical Engineering	

Research Academy Themes:

Highlight which of the Academy's Theme(s) this project will address?
(*Feel free to nominate more than one. For more information, see www.iitbmonash.org)*

1. **Advanced computational engineering, simulation and manufacture**
2. Infrastructure Engineering
3. Clean Energy
4. Water
5. **Nanotechnology**
6. Biotechnology and Stem Cell Research
7. Humanities and Social Sciences

The research problem

Cyclohexane oxidation is one of the most important reactions in the chemical process industry, with more than a million tons of oxidation products (cyclohexanol+cyclohexanone) produced every year. And yet, it is also one of the most inefficient processes, being practiced only to a conversion of 4-8% because of selectivity problems. The main interest in this reaction is therefore to push the conversion-selectivity limits to higher values, and do this in an environmentally friendly way through the use of heterogeneous catalysts. In our previous (recently concluded) work, we have come up with some catalysts which show promise in terms of (i) being able to offer higher selectivities at conversions of industrial interest, and (ii) produce a product that has a high ketone/alcohol ratio, something that is

preferred for ease of further conversion. These catalysts are mixed oxides of cobalt and molybdenum, and synergistically combine the activity of cobalt catalyst with the ketone selectivity of molybdenum. We have also succeeded in supporting these catalysts on mesoporous silica supports. The supported catalysts show higher activity, but a lower ketone selectivity as compared to the unsupported oxides. In this project, we propose to study these features in detail with a view to understanding the mechanism of action as an aid to coming up with better functionality for the supported catalysts. We also aim to study some newer catalysts such as gold, which have been attracting attention in recent literature.

Project aims

1. *To study cyclohexane oxidation with silica-supported $CoMoO_4$ catalyst in a batch slurry reactor and a spinning basket reactor to understand the kinetic features in sufficient detail to enable reactor design.*
2. *To conduct preliminary studies on other catalysts being reported in recent literature as having potential for cyclohexane oxidation*
3. *To identlfy and study suitable reactor-level options from an engineering viewpoint in the light of the kinetic features presented by the catalysts.*

Expected outcomes

1. *One or a series of supported Co-Mo catalysts which are novel and competitive with the best catalysts proposed so far for the reaction*
2. *High impact publications on the kinetics, mechanism, novel catalytic features and engineering aspects of heterogeneous catalysis of cyclohexane oxidation*

How will the project address the Goals of the above Themes?

The project will address a dire need of the chemical manufacturing industry by addressing the efficiency issues in a major industrial reaction from a fundamental angle. The supported catalysts have nanosize particles and it is suspected that their differences with the features of larger size unsupported catalysts are traceable to their nano-size. These investigations will therefore result in contributions to the area of nanocatalysis.

Capabilities and Degrees Required

The ideal student will have –

(i) a masters' degree in chemical engineering with demonstrated expertise in conducting, analysing and modelling chemical reactions and reactors. OR

(ii) a bachelor's degree in chemical engineering with demonstrated aptitude for chemical reaction engineering

Potential Collaborators

Please visit the IITB website www.iitb.ac.in OR Monash Website www.monash.edu to highlight some potential collaborators that would be best suited for the area of research you are intending to float.

Prof Huanting Wang, Department of chemical engineering
Prof Alan Chaffee, Department of chemistry

Please provide a few key words relating to this project to make it easier for the students to apply.

Cyclohexane oxidation, heterogeneous catalysis, gas-liquid-solid reactions