IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Catalytic Conversion of Cellulose and Hemicellulose into Value Added Chemicals**
Project Number	**IMURA0377**

Reliance Industries Limited

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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

The research problem

Increasing CO2 concentration in the atmosphere and the global depletion of easily accessible crude oil

has been a cause of concern for over a decade now. However, clear solutions to obtain high quality and reliable fuels and chemicals from biological feedstock have not yet been found. The development of integrated biorefineries that produce platform chemicals and value added chemicals (low volume high value) in addition to fuels such as ethanol (high volume low value), is of particular interest. However, it requires development of novel processes that can produce value added chemicals, as well as the integration of those novel processes in the integrated biorefinery complex. This research proposal proposes to address this challenge by integrating experimental as well as computational approaches. In particular this project will be focused on converting cellulose and hemicellulose into value added chemicals, and using model based approach to develop optimal reactor design and operational strategies.

Project aims

Process development:

The first aim of this research will be to directly convert the cellulose and hemicellulose into levulinic acid using heterogeneous catalysts based on novel nanomaterials. Levulinic acid is one of the most important platform chemicals which can be converted to fuel additives and chemicals. In the next step the aim will be convert the levulinic acid into a selection of various value added chemicals which can be applied in various industries. The chemicals most important to Australian industries are 2-MethylTetraHydroFuran, γ-Velerolactone, β-Acetylacrylic Acid, Acrylic Acid and Levulinate Esters.

Model based design and optimization:

We will develop a reaction kinetic model for the conversion of cellulose and hemicellulose into value added products through different reaction steps as described above. Using fundamentals of reaction engineering, the model will be developed. The parameters of the model such as the kinetic rate constants and the order of the reaction will be determined from the experimental studies. The model will be parameterized and validated. The validated model will then be used to perform reactor design and optimization. This will subsequently lead to performing a techno-economic analysis of the process option.

Expected outcomes

This project will deliver a great understanding of the catalytic pathways of selective conversion of cellulose and hemicellulose into value added chemicals. A kinetic model will be developed to understand the role of catalysts and reaction conditions on the conversion of cellulose and hemicellulose and the yield and selectivity of the value added chemicals. The model, after validation, will provide optimized reactor configurations and designs. The work will also determine the economic viability of this process.

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

Clean Energy – This project will develop new catalytic process for the industry for cleaner production of value added chemicals. It will also identify the optimal designs of the process of interest to achieve techno-economic feasibility.

Nanotechnology – This project will develop novel catalysts based on nanomaterials such as porous metal oxides, core-shell metal and metal oxide nanoparticles and application of graphene and porous carbon materials as catalysts.

Advanced computational engineering, simulation and manufacture – The kinetic model and the reactor model will provide a platform for future studies of similar systems.

Capabilities and Degrees Required

List the ideal set of capabilities that a student should have for this project. Feel free to be as specific or as general as you like. These capabilities will be input into the online application form and students who opt for this project will be required to show that they can

demonstrate these capabilities.

The student will ideally have experience of research in one or more of the following disciplines - Chemical Engineering, Chemistry, Reaction Engineering, Reactor design; Catalysis and Materials Engineering, Computational (process) modelling, Numerical methods.

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.

Additional costs and equipment

Describe below additional costs that would be needed to complete this project.
This would typically include project-related costs (such as consumables).
Computers, desks, conference travel, student travel to Australia, etc should not be included here. They are already provided for.
IF AMOUNT BEING SOUGHT IS IN EXCESS OF INR 3 lakhs OR $6000, PLEASE COMPLETE FOLLOWING SECTION AS WELL

Equipment required for this project will be provided from the existing lab infrastructure available at IITB and Monash University. The following things are requested in this project –

- Project related consumables such as catalysts precursors and analysis of the projects in LCMS-TOF, HPLC, GCMS and GC will be required.
- Modelling and simulation software may be required

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