IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Designing catalyst- containing industry-ready reactor for facile CO_2 to CO conversion**	
Project Number	**IMURA0988**	
Monash Main Supervisor (Name, Email Id, Phone)	Sankar Bhattacharya Email: Sankar.Bhattacharya@monash.edu	*Full name, Email*
Monash Co-supervisor(s) (Name, Email Id, Phone)	To be decided	
Monash Head of Dept/Centre (Name,Email)	Mark Banaszak Holl Mark.banaszakholl@monash.edu	*Full name, email*
Monash Department:	Chemical Engineering	
Monash ADGR (Name,Email)	Jacek Jasieniak Jacek.jasieniak@monash.edu	*Full name, email*
IITB Main Supervisor (Name, Email Id, Phone)	Arnab Dutta Email: arnab.dutta@iitb.ac.in	*Full name, Email*
IITB Co-supervisor(s) (Name, Email Id, Phone)	Vikram Vishal Email: v.vishal@iitb.ac.in	*Full name, Email*
IITB Head of Dept (Name, Email, Phone)	M. Ravikanth Email: head.chem@iitb.ac.in	*Full name, email*
IITB Department:	Chemistry	

Research Clusters:	**Research Themes:**
Highlight which of the Academy's CLUSTERS this project will address? ***(****Please nominate JUST* ***one.*** *For more information, see www.iitbmonash.org)*	**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	Material Science/Engineering (including Nano, Metallurgy)	**1**	Artificial Intelligence and Advanced Computational Modelling
2	Energy, Green Chem, Chemistry, Catalysis, Reaction Eng ✓	2	Circular Economy
3	Math, CFD, Modelling, Manufacturing	3	Clean Energy ✓
4	CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control	4	Health Sciences
5	Earth Sciences and Civil Engineering (Geo, Water, Climate)	5	Smart Materials
6	Bio, Stem Cells, Bio Chem, Pharma, Food	6	Sustainable Societies
7	Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng		
8	HSS, Design, Management		

The research problem

Since the advent of chemical industrialization (circa 1750), the atmospheric CO_2 level has risen alarmingly by ~1.5 times to reach 411 ppm in the present day. The growth of population and rapid improvement in the life quality coupled has fueled a growth in the CO_2 emission in the developing countries around the world. Following the Paris accord 2015, India has taken the pledge to cut down the annual CO_2 emission by 30% by 2030, acknowledging the negative impact of the ever-growing aerial CO_2 concentration. The conventional energy sector, steel-iron plants, and cement plants are the major contributors to industrial CO_2 emission in India, accounting for ~80% of the anthropogenic CO_2 production. Over the years, the industries have employed several CO_2 capture techniques, including pre-combustion and post-combustion methods to mitigate the direct CO_2 emission to the atmosphere. However, the high cost associated with the existing CO_2 capture methods and the absence of any sustainable long-term utilization plan for the stored CO_2 has severely impeded the natural growth of the heavy CO_2-producing industrial sectors.

Project aims

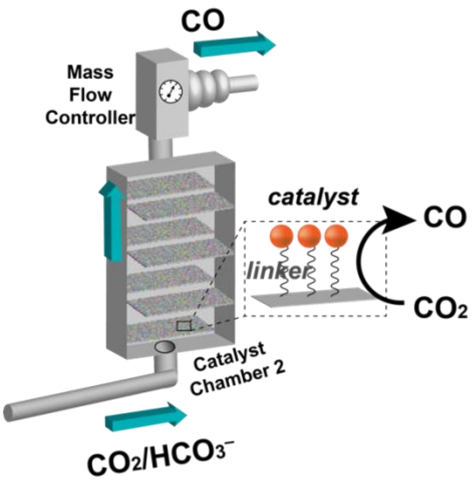
In the proposed project, we are aiming to develop a facile CO_2 to CO convertor unit that can be assembled in an industrial setup establishing a unique approach for CCUS. The final product CO can be employed for fuel (hydrocarbon via Fischer-Tropsch process and alkene via hydroformylation) and bulk chemicals (e.g. acetic acid via Cativa process and detergents via Shell higher olefin process) production in existing industrial processes. This project has two distinct experimental segments, backed by thermodynamic calculations, as follows:

Module 1: *Development of an enzyme design-inspired first-row transition element-based* ***catalyst*** *and employ for an efficient CO_2/CO conversion. The salient features of this module are:*

(i) The ***catalyst*** *will be anchored on a solid surface. An electrically conducting surface will be utilized as the host for electrocatalyst to improve the overall catalytic efficiency.*

(ii) The CO_2 will be charged from the bottom of the chamber with an outlet present on the top to ensure maximum interaction between the ***catalyst*** *and CO_2.*

(iii) ***The catalyst*** *will be active in an aqueous solution; hence, this process can be executed in a sustainable manner without the usage of any organic solvent or hazardous acids.*



Schematic diagram of the CO_2 to CO convertor.

Module 2: *Modifying the reactor design to upscale the CO_2 conversion rate matching the industrial requirement*

(i) The arrangement of the surface-immobilized catalysts will be probed for the maximum CO_2 conversion.

(ii) The flow rate of incoming CO_2 and outgoing CO gas will be regulated properly with a mass flow controller.

(iii) An appropriate temperature and solvent flow controller will be installed along with on-line measurement of CO concentration at exit.

The above experimental data will be used for developing the kinetics of the catalyzed reaction

What is expected of the student when at IITB and when at Monash?

Highlight how the project will gain from the students stay at IITB and at Monash.

The proposed project is evidently an inter-disciplinary project where a student has to initially design a molecular catalyst and probe its reactivity for CO_2 reduction on a bench scale. During this study, the student will learn inorganic and organic synthesis, spectroscopic characterization techniques, electrochemical techniques, and gas analysis methodologies. Then, the student will optimize the catalytic assembly for industry-relevant conditions. This segment of the research work will be executed at IIT Bombay.

In the final section, the student will travel to Prof. Bhattacharya's lab at Monash University and learn the fundamentals of reactor design. Next, the already optimized catalyst will be integrated into a new reactor and will be tested for large-scale CO_2 conversion. The student will upgrade the reactor design following multiple iterations and finally test it for on-site application.

Expected outcomes

Highlight the expected outcomes of the project

(i) Development of a new genre of efficient CO_2 reduction catalyst functional under sustainable conditions.
(ii) Investigate the catalytic mechanism of the catalyst to optimize their operational conditions
(iii) Devising an industry-ready reactor design including the synthetic catalysts
(iv) Optimizing the reactor design for industrial CCUS.

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

Describe how the project will address the goals of one or more of the 6 Themes listed above.

This project directly provides a solution for clean energy theme.

(1) Adaptability: This proposed reactor can be incorporated with other existing CO_2 capture or utilization technologies.

(2) Sustainability: The use of highly efficient catalyst ensures an energy-efficient CO_2/CO conversion that can be executed under ambient conditions in the presence of benign chemicals. The involved catalytic process in this unit predominantly follows green chemical methods to minimize the hazardous waste products.

(3) Waste to wealth: The proposed system will reduce CO_2 while opening up a new avenue for generating revenue by economic production of CO, which already has a thriving industrial demand.

Potential RPCs from IITB and Monash

Provide names of the potential research progress committee members (RPCs) and describe why they are most suited for the proposed project

1. Prof. Anand Rao, CTARA, IIT Bombay
Prof. Rao is an expert on CCUS technology and technology assessment. Hence, his insight will be critical for the designing of the catalysts operational under industry-relevant conditions.
2. Prof. Debabrata Maiti, Chemistry, IIT Bombay
Prof. Maiti is a leading catalyst designer whose inputs will be critical for the development of CO_2 reducing molecular catalysts.
3. Prof. Sanjay Mahajani, Chemical Engineering, IIT Bombay
Prof. Mahajani is renowned for his work in reaction engineering and catalysis. Thus, his involvement in this project will allow the student to grasp the fundamentals of a reactor design.
4. Prof Raman Singh, Chemical Engineering, Monash University. Prof Singh has a strong materials and industry background useful for this project

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.

1. First and foremost, the prospective student should be enthusiastic in solving one of the contemporary global challenges: establishing the carbon-neutral energy economy.
2. The student should have basic knowledge in handling materials, inorganic complexes, and organic solvents.
3. The student should have a master's degree in chemistry or chemical 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.

To be decided

Select up to **(4)** keywords from the Academy's approved keyword list **(available at http://www.iitbmonash.org/becoming-a-research-supervisor/)** relating to this project to make it easier for the students to apply.

1. Water, climate change (Carbon Capture and Sequestration)
2. Green Chemistry and Renewable Energy
3. Catalysis and Reaction Engineering
4. Waste to Wealth