IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Studies on catalyst deactivation during methane conversions**	
Project Number	**IMURA0405**	
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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

Improvement in natural gas conversion efficiency is obviously important. Catalysts play an important role in the technology. The scientific community has put enormous efforts into the study of methane activation since the last couple of decades**.** However, Today only a handful of gas-to-liquid (GTL) plants operated commercially. The reasons for limited GTL facilities are due to the challenged economics, complexity in process operations due to coking and environmental issues**.**

It is, therefore, of great practical importance to understand the mechanism of coke formation and active site

responsible for coke. This study enables us to develop catalysts for this process..

Project aims

To understand catalyst deactivation phenomena during methane conversion

Target reactions

Dry Reforming: $CH_4 + CO_2 \rightarrow 2CO + 2H_2$ $\Delta H = +247$ kJ/mol (Endothermic)

Side reactions in dry reforming

Methane cracking: $CH_4 \rightarrow C + 2H_2$	$\Delta H = 6.3$ kJ/mol
Boudouard reaction: $C + CO_2 \rightarrow 2CO$	$\Delta H = 159.9$ kJ/mol
Reverse water-gas shift reaction: $H_2 + CO_2 \rightarrow CO + H_2O$	$\Delta H = 41.1$ kJ/mol
Carbon gasification: $C + H_2O \rightarrow CO + H_2$	$\Delta H = 131$ kJ/mol
Steam reforming: $CH_4 + H_2O \rightarrow CO + 3H_2$	$\Delta H = 205$ kJ/mol
Dis-proportination reaction: $2CO \rightarrow C + CO_2$	$\Delta H = -159$ kJ/mol

Expected outcomes

- Understanding mechanistic aspect of “C’ formation
- Identify/develop new catalyst composition prone to less ‘C’ formation
- Better understanding of catalyst regeneration technique
- Optimize the operation mode for the reaction

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

Identify the source(s) of ‘C’ present in coke by ^{13}C isotopic investigation

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To understand various types of ‘C’ formation during reaction

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To establish the mechanistic aspect of ‘C’ formation

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To establish deactivation model using molecular modeling tools

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Validation of model using catalyst develop by SABIC (Will be done @ STC-B)

Capabilities and Degrees Required

- Degree: M.Sc in chemistry / M.Tech in chemical engineering
- Basic understanding of catalysis.
- Knowledge on molecular modeling and simulation would be added advantage.
- Basic knowledge in catalyst characterization, gas chromatography & data interpretation
- Familiar with literature search tools and prior art
- Good in technical report writing and communications

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.

For Industry Partners::
Potential Collaborators

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

Major Milestones:

Please add major intended milestones for the project

#	Milestone	Deliverable	Timeline	Responsible
A	• Identify coke source	• Synthesis catalyst • ^{13}C isotopic investigation study		
B	• Identify site/function responsible for various type of coke	• Analyse coke using analytical tools • Establish coke forming mechanism		
C	• Establish mechanistic aspect of coke formation	• Development of deactivation model and validation with experimental data		
D	• Validation of model	• Validation of model using SABIC proprietary catalysts @ STC-B		
E	•			
F	•			