

An Indian-Australian research partnership

Project Title: **Develop a microkinetic model framework for heterogeneously catalyzed reaction – Direct Aromatization of Methane**

Project Number **IMURA0403**

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Chemical

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

Define the problem

- Microkinetic modeling is emerging as a powerful approach to understand complex catalytic reactions.
- In microkinetic modeling, all possible elementary steps comprising the reaction mechanism are considered explicitly. No assumptions on rate-determining step made.
- The microkinetic model incorporates the basic surface chemistry involved in the catalytic reactions.
- The model will have less parameters to estimate and valid over broad operating conditions.
- Such model will be a convenient tool to understand and devise methods to improve catalyst selectivity and stability.

Direct Methane Aromatization – Literature Information

- Catalysts studied and reported in literature – Transition metal/Mo/H-ZSM-5,
- Potential transition metal – Ga, Zn, Pd, Ni, W, Cu, Ru
- Typical product/side reaction species formed are,
 - Ethane
 - Ethylene
 - Propane
 - Benzene
 - Toluene
 - Xylene
 - Napthalene
 - Coke
- Reaction temp: 700 to 850 °C
- Reaction pressure : Sub-atmospheric to 5 bar

Project aims

Define the aims of the project

To develop microkinetic model framework for direct aromatization of methane over zeolite catalysts and validate with literature/experimental data. The Model should validate the kinetic experimental data reported for zeolite catalysts with different metals.

Expected outcomes

Highlight the expected outcomes of the project

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.

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.

- Surface chemistry knowledge as related to catalysis./ design of Catalysts
- Reaction engineering knowledge
- Mathematical modeling knowledge (or knowledge in use of available softwares like ChemKin)

Ideal candidate would be a chemical engineer with heterogeneous catalysis knowledge

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.

