IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Simulation of interfacial properties of gas hydrates for clean energy applications**
Project Number	**IMURA0650**
Monash Main Supervisor (Name, Email Id, Phone)	Nikhil Medhekar, Nikhil.Medhekar@*monash.edu* *Full name, Email*
Monash Co-supervisor(s) (Name, Email Id, Phone)	
Monash Department:	Materials Science and Engineering
IITB Main Supervisor (Name, Email Id, Phone)	Ajay Singh Panwar, panwar@iitb.ac.in *Full name, Email*
IITB Co-supervisor(s) (Name, Email Id, Phone)	
IITB Head of Dept (Name, Email, Phone)	N. Venkataramani *Full name, email*
IITB Department:	Metallurgical Engineering & Materials Science

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

Gas hydrates occur naturally beneath the seafloor near continental edges, and represent a vast reserve of potentially exploitable natural gas; a cubic volume of gas hydrate is estimated to expand to 150 – 180 cubic volumes of gas at standard temperature and pressure. A gas hydrate is a non-stoichiometric crystalline inclusion compound where the basic unit is a hydrogen-bonded hollow cage of host water molecules which contains a single guest gas molecule. Without the inclusion of the guest molecule, the empty lattice is thermodynamically unstable.

Their cage-like structures also make them potential candidates for storage of gases, such as carbon dioxide and hydrogen, thus providing attractive technologies for either carbon dioxide

sequestration (reducing greenhouse gases) or hydrogen storage (clean energy fuel storage). Also, in deep water oil pipelines, hydrate particle formation at the water-gas interface and their subsequent agglomeration into plugs, can lead to blockages in oil flow.

Hence, understanding the interfacial properties of gas hydrates, specifically with respect to cohesion and agglomeration, is critical for developing strategies for both hydrate mitigation in pipelines, and hydrate extraction from sub-seafloor reserves. The aim of the proposed research is to utilize molecular dynamics simulations in conjunction with thermodynamic calculations to understand the interfacial properties of gas hydrates, their cohesion and agglomeration under realistic conditions (for example, -10°C and 300 atm).

Project aims

The project aims to investigate,

1. The mechanisms of cohesion and agglomeration of gas hydrate particles using molecular dynamics simulations.
2. Calculation of interfacial properties of gas hydrate interfaces using molecular dynamics under realistic temperature and pressure conditions: In the absence of reliable gas hydrate interfacial energy data and experimental difficulties involved in obtaining the same, molecular simulations can be used to calculate interfacial properties.

Such knowledge is vital for not only preventing hydrate formation in pipelines, but also for exploiting hydrates as alternate sources of hydrocarbons.

Expected outcomes

i) Implementation of parallel molecular dynamics simulation and numerical methods for estimation of interfacial properties of gas hydrates

ii) Understanding the interfacial mechanisms related to gas hydrate cohesion and agglomeration

iii) Generation of interfacial energy data for gas hydrates at both gas/solid and liquid/gas hydrate interfaces

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

The proposed research justifies the above mentioned goals in the following ways,

1. Clean energy: Gas hydrates are potential candidates for both carbon dioxide and hydrogen storage.
2. Alternate sources of energy: Gas hydrates represent a very large natural gas resource.
3. Advanced simulation and thermodynamic calculation methods will be utilized for calculation of properties.
4. Understanding of interfacial properties and agglomeration processes are critical for all nanotechnology applications.

Capabilities and Degrees Required

Candidates with the following degrees, either a M. Tech. or an exceptional B. Tech. degree in Engineering (Metallurgical Engineering, Materials Science & Engineering, Mechanical Engineering or Chemical Engineering) or M.Sc. in either Physics or Chemistry, will be suitable for the project.

Candidates should have excellent mathematical aptitude, good programming and numerical skills.

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.

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

Simulation, Clean energy, Interfacial science