IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	Techno-economic evaluations of solar (or other advanced technologies) for splitting water for hydrogen and oxygen feedstock to ammonia and nitric acid production
Project Number	**IMURA0222**

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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

Producers of industrial chemicals such as ammonia increasingly have a responsibility to investigate methods where the products have less impact on the environment. Ammonia is produced from hydrogen and nitrogen. Syngas provides the source of hydrogen gas for reaction with nitrogen gas to form anhydrous ammonia. Syngas is a mixture of hydrogen, carbon monoxide and carbon dioxide that is commonly produced by reforming natural gas in the presence of steam over a metal alloy catalyst, which is usually nickel based. This process is known as steam reforming of natural gas. The natural gas is mixed with combustion air and burned to produce heat inside a reformer unit, before waste heat is removed from the flue gas which is vented to atmosphere. The flue gas emits carbon dioxide, and along with the carbon dioxide that is removed from the process gas stream post hydrogen production, these emissions constitute the major greenhouse gas emissions from an online ammonia manufacturing plant. The natural gas used in ammonia manufacture constitutes the vast majority of operating costs so any method that reduces the dependence on this hydrocarbon could also have a significant impact of plant economics

Renewable fuels and feedstocks may offer the opportunity to reduce costs and the overall carbon dioxide emissions. This project will look at processes based on solar (or other advanced technologies) for splitting water for hydrogen and oxygen feedstock to ammonia and nitric acid production. A fairly large scale of operation will be used as the basis for these studies.

Relevant Background and additional information:

The project is expected to involve a mix of heat and mass balance-based process flow modelling, supplemented by experimental analysis to generate understanding of likely gas and pollution composition ranges. Appropriate gas-separation experiments may also be conducted.

Relevant literature:

Ulgiati, S., Raugei, M., and Bargigli, S., (2006), Overcoming the inadequacy of single-criterion approaches to Life Cycle Assessment, *Eco. Mod*., **190**, 3-4, 432-442.

Dominguez-Ramos, A., Aldaco, R., and Irabien, A., (2007), Life Cycle Assessment as a Tool for Cleaner Production: Application to Aluminium Trifluoride, *Int. J. Chem Reaction Engng.,* **5**, A33.

Project aims

To identify and assess leading technologies for hydrogen generation from water splitting in the generation of ammonia from syngas feedstock, with the inclusion of CO2 capture. The project is expected to involve a mix of heat and mass balance-based process flow modelling, supplemented by experimental analysis of water splitting to generate understanding of likely gas and pollution composition ranges. Appropriate gas-separation experiments may also be conducted. The study is expected to enable the identification of the most fruitful avenues to pursue in greater detail.

Expected outcomes

Highlight the expected outcomes of the project

The project outcomes are expected to provide:

- an analysis of possible technologies for hydrogen generation through the water splitting;
- comparison of the economic and environmental credentials of existing routes for ammonia production with those of alternate flowsheets involving hydrogen production via water splitting;
- a completed program of experimental work characterizing outputs, and efficiency of promising technologies capable of integration into ammonia production.

Capabilities and Degrees Required

Essential: Masters in Chemistry or Chemical Engineering

Desirable: Experience in CO2 capture

Desirable: Experience in catalysis and electrochemistry