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2.5 Objective of the research work

This thesis aims to select novel aqueous amine blends and study their performance for post-combustion CO_2 capture. The overall point-wise objectives of this thesis work are as follows:

- The prime objective of this thesis work is to evaluate CO_2 absorption-desorption performance for the selected novel aqueous amine blends of BAE+DMAE, HMDA+DMAE, and TETA+DMAE for post-combustion CO_2 capture.
- The first objective is validating the experimental setup and estimating equilibrium CO_2 loading during CO_2 absorption investigation.
- Analyzing the effect of process parameters on equilibrium CO_2 loading as per the chosen range of operating conditions.
- Developing an empirical model for the validation of CO_2 absorption results.
- To evaluate the cyclic capacity, cyclic equilibrium CO_2 loading, heat duty, and regeneration efficiency of the novel blends and their comparison with the benchmark MEA during the CO_2 desorption study.
- To examine pH, density, CO_2 absorption and desorption rates.
- Proposing reaction mechanism for novel aqueous amines of BAE+DMAE, HMDA+DMAE, and TETA+DMAE when reacting with CO_2 and their validation by ^{13}C NMR and FTIR characterization.
- To study the heat of CO_2 absorption (ΔH_{abs}) for all novel aqueous amine blends.
- Modeling and optimization of equilibrium CO_2 loading by the RSM software.
- To study the toxic behavior of the chosen novel amine blends.

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List of Publications

Patent filed:

Monoj Kumar Mondal and **Ashish Gautam**. An aqueous amine blend for post-combustion capture (**Application number: 202411034454).**

Publications in Science Citation Indexed (SCI) Journals:

1. **Ashish Gautam** and Monoj Kumar Mondal. Post-combustion CO_2 absorption-desorption performance of novel aqueous binary amine blend of Hexamethylenediamine (HMDA) and 2-Dimethylaminoethanol (DMAE). *Energy* (*Elsevier Publication*) **2024**; 296: 130982. (**Impact factor = 9**)
2. **Ashish Gautam** and Monoj Kumar Mondal. Novel aqueous amine blend of 2-(Butylamino) ethanol and 2-Dimethylaminoethanol for CO_2 capture: Equilibrium CO_2 loading, RSM optimization, desorption study, characterization and toxicity assessment. *Separation and Purification Technology* (*Elsevier Publication*) **2023**: 322: 124279. (**Impact factor = 8.1**)
3. **Ashish Gautam** and Monoj Kumar Mondal. Post-combustion capture of CO_2 using novel aqueous Triethylenetetramine and 2-Dimethylaminoethanol amine blend: equilibrium CO_2 loading-empirical model and optimization, CO_2 desorption, absorption heat, and ^{13}C NMR analysis. *Fuel* (*Elsevier Publication*) **2023**; 331: 125864. (**Impact factor = 6.7**)
4. **Ashish Gautam** and Monoj Kumar Mondal. Review of recent trends and various techniques for CO_2 capture: Special emphasis on biphasic amine solvents. *Fuel* (*Elsevier Publication*) **2023**; 334: 126616. (**Impact factor = 6.7**)

5. Akhil Kumar Gupta, **Ashish Gautam**, and Monoj Kumar Mondal. Experimental, modeling and RSM optimization of CO_2 loading for an aqueous blend of Diethylenetriamine and 3-Dimethyl amino-1-propanol. *Korean Journal of Chemical Engineering* (*Springer Publication*) **2023**; 40(5): 1151-67. (**Impact factor = 2.9**)

Book chapters:

1. **Ashish Gautam** and Monoj Kumar Mondal. Chapter: Recent advances in Microalgae process for post-combustion CO_2 capture (**Book**: Microbial Niche Nexus Sustaining Environmental Biological Wastewater and Water-Energy-Environment Nexus – By *Springer*) (**Accepted**).
2. **Ashish Gautam** and Monoj Kumar Mondal. Chapter 16: Algal bioplastics/ Polyhydroxybutyrate production: algal diversity, biosynthetic pathways, extraction methods and technical aspects, current prospects/applications, market trends (**Book**: Algae-derived Biochemicals of Industrial Importance – By *Springer Cham*) (**Accepted**).
3. **Ashish Gautam** and Monoj Kumar Mondal. Chapter 10: Scope of Food Waste to Resource Recovery: A Way of Green Advocacy (**Book**: Resource Recycling and Management of Food Waste – By *Springer Nature*) (**Communicated for publication**).

International conferences:

1. **Ashish Gautam** and Monoj Kumar Mondal. 2-(Methylamino)ethanol and 2-Dimethylaminoethanol aqueous amine blend for post-combustion CO_2 capture– Targeting net-zero emission. **IIChE-CHEMCON**, organized by **Heritage Institute of Technology, Kolkata** during 27-30 December, 2023.

2. **Ashish Gautam** and Monoj Kumar Mondal. Aqueous amine blend of 1,4-Butanediamine and 2-Dimethylaminoethanol for post-combustion CO_2 capture: An approach towards carbon neutrality. **ICPHD**, organized by **IIT Guwahati** during 03-05 November, 2023.
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4. **Ashish Gautam** and Monoj Kumar Mondal. Aqueous Piperazine (PZ) and 2-Dimethylaminoethanol (DMAE) amine blend for post-combustion CO_2 capture: Absorption and desorption study. **CHEM-TECHNOVA**, organized by **HBTU, Kanpur** during 26 to 27 May, 2023.
5. **Ashish Gautam** and Monoj Kumar Mondal. Aqueous Triethylenetetramine and 3-Dimethylamino-1-propanol amine blend for post-combustion CO_2 capture. **CHEMCON**, organized by **HBTU, Kanpur** during 27-30 December, 2022. (**Best oral presentation award**)
6. **Ashish Gautam** and Monoj Kumar Mondal. Triethylenetetramine and 2-(Diethylamine)ethanol aqueous amine blend for Post-combustion CO_2 capture. **CHEMSMART**, organized by **NIT, Rourkela** during 16-18 December, 2022.
7. **Ashish Gautam** and Monoj Kumar Mondal. 1,5-Diamino-2-methylpentane and 2-Dimethylaminoethanol aqueous amine blend for post-combustion CO_2 capture. **ABC-HEE**, organized by **MNNIT Allahabad, Prayagraj** during 20-22 October, 2022.

8. **Ashish Gautam** and Monoj Kumar Mondal. Aqueous Triethylenetetramine and 2-Dimethylaminoethanol amine blend for post-combustion CO_2 capture: Equilibrium CO_2 loading, desorption study, empirical modeling and ^{13}C NMR analysis. **CHEMTSF**, organized by **IIT, Roorkee** during 8-10 September, 2022.

Workshops and Training programs:

1. National Training Program on "Water Urbanism for Resilient Development: Case Studies from Varanasi, India" organized by **IIT (BHU)** and **National Institute of Disaster Management** (**NIDM**) New Delhi, (**Ministry of Home Affairs, Govt. of India**) on 04-06 September, 2023.
2. **LaTeX** - Introductory workshop organized by Teaching and Learning cell, **IIT (BHU), Varanasi**, India on 15 April, 2023.