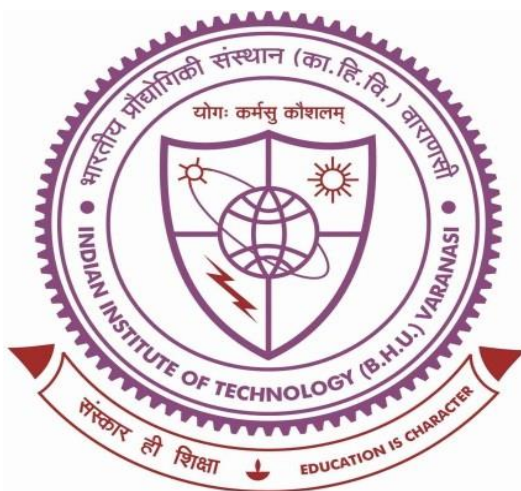


**Post-combustion CO<sub>2</sub> capture by using novel  
BAE+DMAE, HMDA+DMAE and  
TETA+DMAE aqueous amine blends**



Thesis submitted in partial fulfillment

for the award of degree

of

**Doctor of Philosophy**

By

*Ashish Gautam*

**Department of Chemical Engineering & Technology  
Indian Institute of Technology  
(Banaras Hindu University)  
Varanasi – 221005, India**

**Roll No. 19041007**

**2024**

# Chapter 6

## Overall Conclusion and Future Recommendations

---

### 6.1 Overall conclusion

This chapter summarizes the overall conclusion of the research conducted over novel aqueous amine blends for post-combustion CO<sub>2</sub> capture. The point-wise overall conclusions of this thesis research work are as follows:

- ❖ Novel aqueous amine blends of BAE+DMAE, HMDA+DMAE, and TETA+DMAE showed promising results during CO<sub>2</sub> absorption and desorption investigation.
- ❖ The maximum equilibrium CO<sub>2</sub> loading ( $\alpha_{\max}$ ) of novel amine blend BAE+DMAE at T = 313.15 K, HMDA+DMAE at T = 298.15 K, and TETA+DMAE at T = 315.65 K was found to be 0.9365, 1.2174, and 0.92 mol CO<sub>2</sub>/mol amine, respectively. Novel blends exhibited much higher  $\alpha_{\max}$  value than conventional MEA and previously reported amines and their various blends.
- ❖ The experimental results were validated through developed empirical model and % AARD of BAE+DMAE, HMDA+DMAE, and TETA+DMAE novel amine blends was found to be 3.41, 3.06, and 5.631 %, respectively. The developed modeling equation is highly reliable, accurate and realistic.
- ❖ Experimental investigation revealed that increasing the CO<sub>2</sub> partial pressure and activator's mole fraction increases the CO<sub>2</sub> loading, whereas declining trends in CO<sub>2</sub> loading was observed while increasing temperature and solution concentration.

- ❖ Heat of CO<sub>2</sub> absorption ( $\Delta H_{\text{abs}}$ ) of novel blends of BAE+DMAE, HMDA+DMAE, and TETA+DMAE were found to be  $-72.74$ ,  $-75.50$ , and  $-67.135$  kJ/mol, respectively. These values are lower than MEA, suggesting lower regeneration heat duty demand.
- ❖ The cyclic capacity of novel BAE+DMAE, HMDA+DMAE, and TETA+DMAE amine blends were 71.23, 61.77, and 55.03 % higher than 30 wt% traditional MEA, respectively. High cyclic capacity demands small size of CO<sub>2</sub> capture unit and low solvent circulation rate is needed that finally diminishes the overall cost.
- ❖ Density for CO<sub>2</sub>-unloaded and CO<sub>2</sub>-regenerated amine samples were nearly similar for HMDA+DMAE amine blend, whereas density increment was seen for CO<sub>2</sub>-loaded samples. Density of amine samples was also depending upon amine concentrations.
- ❖ Reduction in heat duty of regeneration for 3 mol/L amine blend solution of BAE+DMAE and HMDA+DMAE as compared with 30 wt% MEA was found to be 74.89 and 70.83 %, respectively.
- ❖ Regeneration efficiency for 3 mol/L amine blend solution of BAE+DMAE and HMDA+DMAE was found to be 83.27 and 60.47 %, respectively.
- ❖ Low regeneration heat duty and high regeneration efficiency of these novel blends reduces the overall operational cost of the entire process.
- ❖ pH for CO<sub>2</sub>-unloaded, CO<sub>2</sub>-loaded, and CO<sub>2</sub>-regenerated HMDA+DMAE amine blend fall in the range of 12.04–12.78, 8.37–9.50, and 9–11, respectively.
- ❖ The initial absorption rate for HMDA+DMAE amine blend for 2 mol/L HMDA–1 mol/L DMAE was  $26 \times 10^{-4}$  mol CO<sub>2</sub>/(L solution. min), yielded a 62.5 % higher absorption rate than 30 wt% MEA. Similarly, initial CO<sub>2</sub>-desorption rate for 0.5 mol/L HMDA–2.5 mol/L DMAE was 43.75 % higher than the benchmark 30 wt% MEA.

- ❖  $^{13}\text{C}$  NMR and FTIR characterization perfectly authenticated the proposed reaction mechanisms for novel aqueous amine blends.
- ❖ RSM provided the maximum equilibrium  $\text{CO}_2$  loading at optimized process parameters.
- ❖ According to toxicity assessment, the novel aqueous amine blends of BAE+DMAE, HMDA+DMAE, and TETA+DMAE are least harmful for the environment.
- ❖ On deeply investigating all three novel blends by focusing on different parameters such as equilibrium  $\text{CO}_2$  loading, cyclic capacity, regeneration efficiency, heat of  $\text{CO}_2$  absorption, and toxicity assessment, it is concluded that the TETA+DMAE amine blend is the best amine blend among all.
- ❖ It is finally concluded that the novel aqueous amine blend of BAE+DMAE, HMDA+DMAE, and TETA+DMAE is recommended for large scale processes to capture  $\text{CO}_2$  from the industrial flue gas stream. However, among these tested blends, the TETA+DMAE amine blend is the most suitable amine blend for industrial applications.

## 6.2 Future recommendations:

Based on the overall conclusion of the present thesis work, some suggestions can be recommendations for future work:

- ❖ More novel DMAE-based aqueous amine blends with commendable  $\text{CO}_2$  absorption and desorption performance can be further explored.
- ❖ Biphasic amine solvents can be focused and in depth characterization can be performed.
- ❖ Based on novel amine blends, large-scale pilot studies can be conducted to capture  $\text{CO}_2$  from the flue gas stream.

- ❖ Thermodynamic modeling such as KE model, modified KE model, NRTL model, Peng-Robinson model etc. can be adopted for modeling purposes.
- ❖ Reaction rate kinetics and mass transfer coefficients can be calculated.
- ❖ Experimental setup can be modified to work under continuous operations.
- ❖ Utilizing solar energy to regenerate the CO<sub>2</sub>-loaded amine blends is an excellent option to reduce the entire operational cost.
- ❖ In depth investigation of desorption study for novel amine blends can be targeted.
- ❖ Cost estimation can be done for CO<sub>2</sub> absorption and desorption experiments.
- ❖ Artificial neural network (ANN), machine learning (ML) and artificial intelligence (AI) are emerging techniques that can be employed to predict the CO<sub>2</sub> loading in the aqueous amine blends.