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_2 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_2 absorption and desorption investigation.
- The maximum equilibrium CO_2 loading (α_{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_2/mol amine, respectively. Novel blends exhibited much higher α_{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_2 partial pressure and activator's mole fraction increases the CO_2 loading, whereas declining trends in CO_2 loading was observed while increasing temperature and solution concentration.

- Heat of CO_2 absorption (ΔH_{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_2 capture unit and low solvent circulation rate is needed that finally diminishes the overall cost.
- Density for CO_2-unloaded and CO_2-regenerated amine samples were nearly similar for HMDA+DMAE amine blend, whereas density increment was seen for CO_2-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_2-unloaded, CO_2-loaded, and CO_2-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 26×10^{-4} mol CO_2/(L solution. min), yielded a 62.5 % higher absorption rate than 30 wt% MEA. Similarly, initial CO_2-desorption rate for 0.5 mol/L HMDA–2.5 mol/L DMAE was 43.75 % higher than the benchmark 30 wt% MEA.

- ^{13}C NMR and FTIR characterization perfectly authenticated the proposed reaction mechanisms for novel aqueous amine blends.
- RSM provided the maximum equilibrium 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 CO_2 loading, cyclic capacity, regeneration efficiency, heat of 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 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 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 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_2-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_2 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_2 loading in the aqueous amine blends.