Modeling of Amine Solutions Reacted with CO_2

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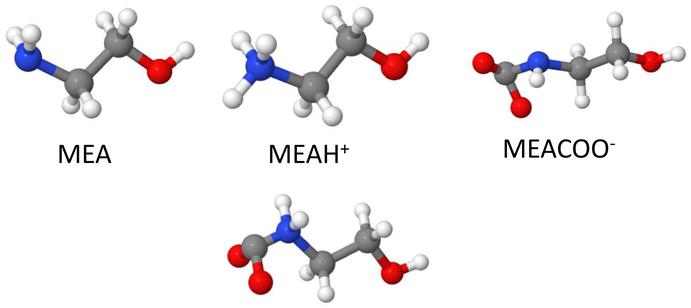
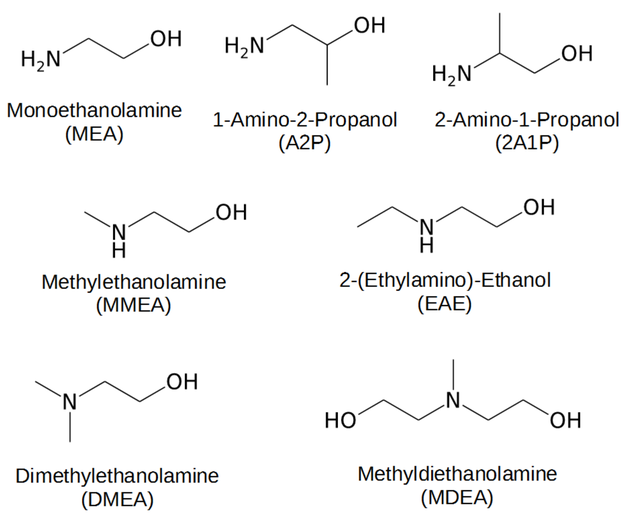
Introduction

- Amine absorbs CO_2 by forming carbamate ion and protonated amine. Some zwitterions are also observed

$$CO_2 + 2RNH_2 \rightleftharpoons RNHCOO^- + RNH_3^+$$

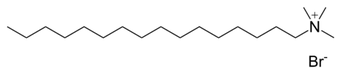


- Aqueous monoethanolamine (MEA) is mostly used for CO_2 capture, but many other amines are also available

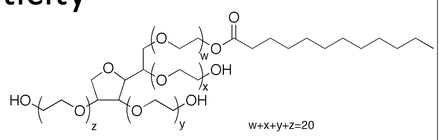


- Which one or which blends are optimum?

- Surfactants added to amine solutions enhance the CO_2 capture rate, but may also lead to foaming problems
- To this end, we need to study their interfacial properties: surface tension and surface elasticity



Cetrimonium Bromide (CTAB)



Tween-20

Methods

- We use molecular dynamics simulations to study the physical properties of aq. amine solutions
- Varying the number of molecules of amine and its derivatives gives varied carbon loadings:

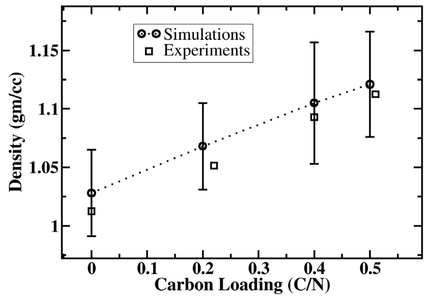
Number of molecules in simulation box

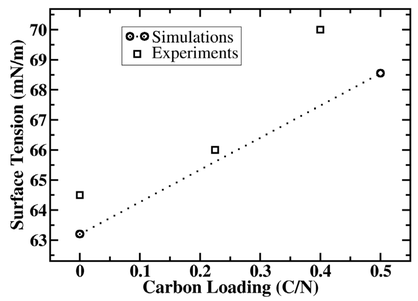
System 1	System 2
960 MEA 7585 water	50 MEA 430 $MEAH^+$ 430 $MEACOO^-$ 50 MEA^+COO^- 7585 water
Corresponds to 30 wt.% MEA (aq.)	Assuming ~ 50% of MEA reacted with CO_2

- Study of amines with 20% and 40% carbon loadings are in progress
- MEA systems were studied; A2P, 2A1P, MMEA, EAE, DMEA are in progress
- Surfactants were added with varying surface loadings

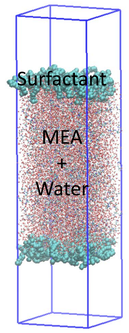
Results

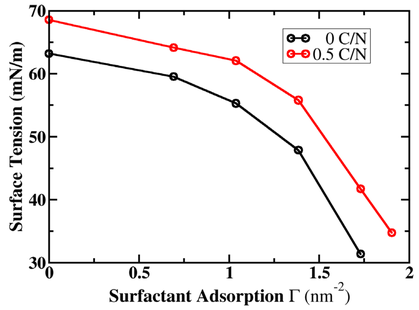
30 wt.% MEA (aq.) at 298 K and 1 atm



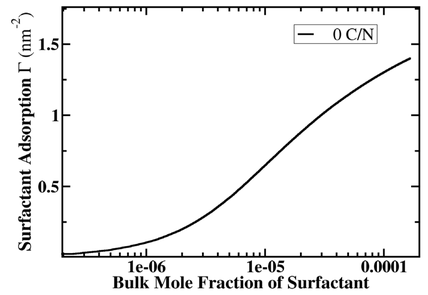


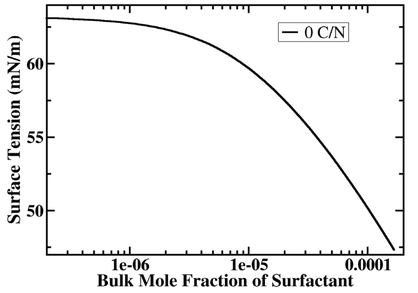
Effect of Surfactants





Results shown for CTAB





Conclusions

- Densities and surface tension of amine solutions increase with increased carbon loading
- Surface tension of solution decreases with increasing the surfactant concentration
- Molecular simulations give insight at a molecular level and predictions, which can help develop better blends

References
- Sresht et al, Langmuir 33.33 (2017): 8319
- Tiwari et al, Submitted to Industrial & Engineering Chemistry, Under Review
- Liu et al, Private Comm., CAER, University of Kentucky

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