Prediction of Foaming Based on Atomistic Simulations of Amine-Based CO_2 Capture Solvents

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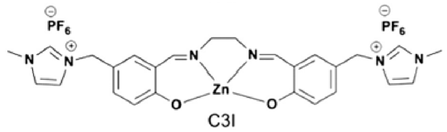
CO_2 Capture using Solvents

- Traditionally, aqueous amine solutions are used for CO_2 capture
- Aqueous amine solutions are not very efficient, and add too much cost for electricity generation, and high capital cost
- Scientists at University of Kentucky have developed special catalysts, which in aqueous MEA solutions increase the CO_2 absorption rate by ~30%, which significantly saves the capital cost
- However, some catalysts exhibit foaming problems and the extent of foaming varies over a series of developed catalysts



C3I

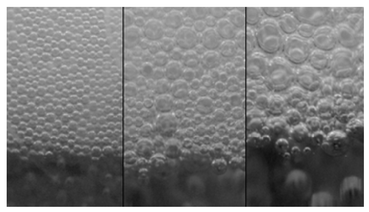
A sample catalyst [2]

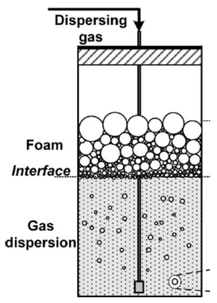
The 0.7 MWe slipstream testing facility

A packed bed column for CO2 absorption [1]

Foaming is Undesired in Absorption Column

- Foams are soapy, kinetically stable bubbles separated by thin films, stacked on the top and in the amine
- Foaming causes
  - Poor absorption of gas
  - High amine losses, carryover in knockouts
  - High capital costs





Empirical Foaming Models

- Foaming models available in the literature
  - Correlate the foam height with various bulk solution properties. E.g. [3]

$$H_0 = 4394 \frac{\gamma}{r_0^{1.60}} \left(\frac{(\mu_l j)^{0.30}}{((\rho_l - \rho_g) g)^{1.30}} \right)$$

- These models miss Interface region properties, which are important in our project because
  - Surface modulus, which determines the film stability, is missed in this model
  - Solution surface tension, viscosity, and density will not change by adding very small amount of catalysts (10^{-5} mole fraction) in MEA solution

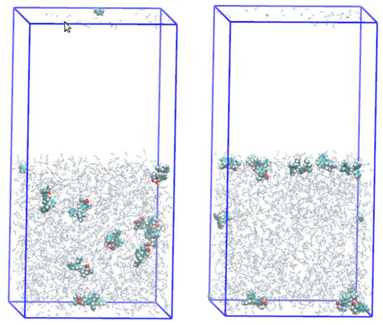
Molecular Dynamics (MD) Simulations

- MD simulations can be used to study interfacial regions
- Simulation details:
  - MEA model by *Hwang et. al.* [4]
  - GAFF for catalysts, charges from *ab-initio* RESP
  - SPC/E water model

MD simulation of interface region

15800 water
+
2000 MEA
+
10 catalysts

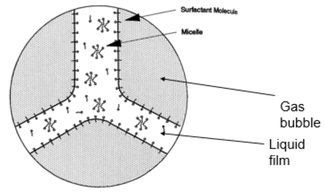
Box length ~ 8 x 8 x 16 (nm)
Initially equilibrated in ~ 8 x 8 x 8 (nm)



Initial Final

- Catalysts tend to come near the surface
- This is because of them having polar and non-polar groups

Catalysts Behave as Surfactants



- Surfactants lower the surface tension
  - Bubbles are easily formed
- When surfactants concentrate in a monolayer at the surface: increased interfacial viscosity and increase surface modulus
  - Provides mechanical resistance to film thinning and rupturing: makes foam more stable

Comparing Two Catalysts

- A and B are two identical molecules except B has N=C compared to A which has H-N-C
- Following properties are calculated from simulation of bulk catalysts at 800 K

Properties	A	B
Bulk modulus (GPa)	2.09	1.39
Viscosity (mPa.s)	5	2
Surface Tension (mN.m)	20.2	16.7
Density (kg/m^3)	879	856
Hydrogen Bonding	More	Less
Experimental Findings	More Foaming	Less Foaming

Summary

- Catalysts increase the CO_2 absorption rate, but some of them create foaming problems
- Catalysts act as surfactants
  - In this way even a small quantity of surfactants affect the foaming
- Interfacial region plays an important role in affecting the foaming

References

1. http://www.netl.doe.gov/research/coal/project-information/proj?k=FE0007395
2. Catal. Sci. Technol. 2014, 4, 3620–3625
3. Colloids and Surfaces A: Physicochem. Eng. Aspects 349 (2009) 125–136
4. Phys. Chem. Chem. Phys., 2015, 17, 831--839