Prediction of Foaming Based on Atomistic Simulations of Amine-Based CO₂ Capture Solvents

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CO₂ Capture using Solvents

• Traditionally, aqueous amine solutions are used for CO₂ 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 CO₂ 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

Empirical Foaming Models

• Foaming models available in the literature
  ➢ Correlate the foam height with various bulk solution properties. E.g. 3
  \[
  H_0 = 4394 - \frac{1}{1.66} \left( \frac{(\mu_j)^{0.30}}{(\rho_l - \rho_g)^{1.30}} \right)
  \]
  • 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

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

<table>
<thead>
<tr>
<th>Properties</th>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk modulus (GPa)</td>
<td>2.09</td>
<td>1.39</td>
</tr>
<tr>
<td>Viscosity (mPa.s)</td>
<td>5</td>
<td>2</td>
</tr>
<tr>
<td>Surface Tension (mN.m)</td>
<td>20.2</td>
<td>16.7</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>879</td>
<td>856</td>
</tr>
<tr>
<td>Hydrogen Bonding</td>
<td>More</td>
<td>Less</td>
</tr>
<tr>
<td>Experimental Findings</td>
<td>More Foaming</td>
<td>Less Foaming</td>
</tr>
</tbody>
</table>

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

Summary

• Catalysts increase the CO₂ 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