Simulation and validation of CO$_2$ mass transfer processes in aqueous MEA solutions with Aspen Plus at CO$_2$ Technology Centre Mongstad

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Outline

• Introduction
  • CO₂ Technology Centre Mongstad

• Experimental
  • Amine plant absorber specifications
  • MEA campaigning (2013/2014 and 2015)
  • Aspen Plus modeling work at TCM

• Results and discussion
  • Overall simulation results
  • Temperature absorber profiles
  • CO₂ loading and enhancement factor absorber profiles
  • Driving forces and flux absorber profiles

• Concluding remarks

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CO₂ Technology Centre Mongstad

• Located at the Mongstad industrial site
  • Oil refinery (flue gas with ~13% CO₂)
  • Gas fired power plant (flue gas with ~3.5% CO₂)

• Amine plant
  • Design & construction: Aker Solutions and Kværner
  • Campaigns: Aker Solution, Shell Cansolv

• Chilled ammonia plant
  • Design & construction: Alstom
  • Campaigns: Alstom

• TCM Owners: Gassnova (Norwegian state), Statoil, Shell, Sasol
• Purpose of TCM is to test, verify, and demonstrate CO₂ removal technologies
  • TCM does not develop CO₂ removal technologies

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TCM Amine plant

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TCM Amine plant – absorber

- Absorber results are well suited for simulator verification (e.g. Aspen Plus)
- Verifies (and tunes) mass transfer/kinetic and equilibrium correlations

- Absorber structure
  - 62 meter total height
  - 3.55m x 2m = 7.1m² cross sectional area
  - Koch Glitsch structured stainless steel packing
    - 3m + 3m = 6m water wash section
    - 12m + 6m + 6m = 24m absorption section
  - Collector trays and redistributors
  - Space available for (future) intercooler connections
  - 3m absorber sump
  - Demisters upstream and downstream water wash sections

- Instrumentation & sampling ports
  - 4 temperature sensors in radial plane at ~1m elevations
  - Solvent sampling stations at solvent inlet, outlet, and between sections
  - Differential pressure sensors over each section
  - Gas and liquid flow meters at inlet and outlet flows

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MEA campaigns at TCM

- TCM conducted MEA campaigns;
  - Dec 2013 – Feb 2014 (in collaboration with Aker Solutions)
  - July 2015 – present (gas phase instrumentation heavily upgraded, results not considered here)

- MEA concentrations ranging 30 – 40 wt% on CO₂ free basis
  - Varying concentration causes different absorber temperature and mass transfer profiles \(\rightarrow\) ideal for simulator verifications

- Purpose of MEA campaigns;
  - Generate baseline results for comparison to commercial vendor technologies
  - Generate non-confidential results for easier and more straight-forward publishing, sharing, and knowledge build-up
  - Etc.
Aspen Plus modelling at TCM

- TCM is using commercial available Aspen Plus simulator
  - Version 7.0, 7.1, 7.3, and now upgrading to 8.6
  - Developed Excel tool for easier user interface with Aspen Plus v7.x
  - Adjustments to the physical solubility of CO₂ and refitted thermodynamic interaction parameters in v7.3 (collaboration with NTNU)
    - No further internal simulator development

- Simulator flow sheet resembles plant as much as possible
  - Heat exchanger coupled absorber/stripper, water wash sections, 2 stripper, and vapor compressors system, etc. implemented
  - Bravo et al. mass transfer/liq hold-up correlation, Chilton & Colburn heat transfer correlation, RadFrac/eNRTL mass transfer/thermodynamic model, etc.
  - Simulation procedure:
    - Input: gas inlet temp & flow, liq. inlet flow & \(a_{CO_2}\), MEA conc., capture rate, and packing height.
    - Model tuning by interfacial area factor \(\rightarrow\) here: 0.55
Absorber modelling and analysis

- **Reactive gas-liquid mass transfer processes simplified:**
  \[ A_{gas} + B_{liq} \rightleftharpoons C_{liq} + D_{liq} \]

- **Assume:**
  - Mass transfer resistance at both gas and liquid side.
  - Reactive mass transfer (kinetics) can be described by the enhancement factor \( E \).
  - Physical gas solubility described by partition coefficient \( m \) and assumption of equilibrium at interface \( i \).

- **Well-known mass transfer relations:**
  - Liquid side mass transfer;
    \[ J_A = k_L \cdot E \left( \frac{c_A^{liq}}{m} - c_A^{liq} \right) \]
  - Gas side mass transfer;
    \[ J_A = k_G \cdot (c_A^{g} - c_A^{liq}) \]
  - Combining and rearranging yields;
    \[ E = \frac{J_A m}{(c_A^{g} - mc_A^{liq} - \frac{J_A}{k_G})_b} \]

- **At each discretization stage, enhancement factor \( E \) and flux can be determined**
  - Provides the rate of absorption into a reactive solvent to the rate into a non-reactive/physical solvent.
Absorber modeling results

- Overall absorber modeling input & results

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>30 wt% MEA</th>
<th>40 wt% MEA</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>Plant</td>
<td>Simulation</td>
</tr>
<tr>
<td>Flue gas flow rate</td>
<td>Sm³/hr</td>
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<td>46.600</td>
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<tr>
<td>Flue gas CO₂ conc. (CHP)</td>
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<td>Depleted flue gas CO₂ conc.</td>
<td>[vol%]</td>
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<td>Capture rate</td>
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<td>Solvent flow rate</td>
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<td>Rich solvent loading</td>
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<td>Packing height</td>
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<tr>
<td>Anti-foam injected</td>
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</tr>
</tbody>
</table>
Results – temp profiles 30 and 40 wt%

- Good temperature predictions
- 40 wt% → higher temp as more CO₂ absorbs → exothermic rxn.
Results – $\alpha_{CO₂}$ and E profiles 30 and 40 wt%

- OK $\alpha_{CO₂}$ prediction $\rightarrow$ mass transfer models may need further improvement
- Reactive chemical MEA absorbent provides highest “impact” on mass transfer at absorber top

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Results – driv. forc., flux profiles 30 and 40 wt%

- Good driving forces throughout, highest flux and driving forces in middle of absorber
  - Top approaching equilibrium due to very low CO₂ gas content → importance of good gas phase instrumentation at absorber to avoid top pinching
  - Bottom approaching equilibrium due to increased P_{CO₂} VLE due to increase $\alpha_{CO₂}$
- Simulated (!) driving force pattern 40 wt% differs → should look similar from exp. $\alpha_{CO₂}$ profile

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Concluding remarks

• Amine plant/absorber at TCM is suited for simulator verifications
  • Temperature and $\alpha_{\text{CO}_2}$ loading profiles are essential → preferably also CO$_2$ gas phase profiles

• A simulator is a good tool for understanding mass transfer when compared to experimental data
  • Highest flux occurs in the middle of the absorber column, pinching to be avoided
  • Further model development essential
    • Mass transfer correlations
    • Higher MEA concentration ranges
  • Simulator temperature profile match is not sufficient for complete description of the mass transfer process

• Further testing necessary
  • Increased CO$_2$ flue gas content → RCC gas with 13-15% CO$_2$
Thank you for your attention!!!

Questions???

Acknowledgments to TCM DA owners

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New sample line

WP2a
WP2b
WP3

Current analyzers

Analyzer
Container (UIO)
PTR-TOF
(NH₃, aldehydes, amines)

New sample line

PTR-QMS 300
Amine
Analyzer House

Amine Absorber Outlet

Analyzer House

3 new sample lines

FTIR
CO₂, NH₃, Aldehyde, amine, etc

GC
CO₂, O₂, N₂, H₂O

IR
CO₂ (0-1 vol%)

IR
CO₂ (0-10 vol%)

IR
CO₂ (85-100 vol%)

O₂
CO₂ (Current)

O₂
Analyzer (0-25 vol%)

O₂
Current

CO₂
Current

CHP/RCC - inlet

GC
CO₂, O₂, N₂, H₂O

FTIR
CO₂, NOₓ, SDx, etc

O₂
CO₂ (0-25 vol%)

IR
CO₂ (0-5 vol%)

IR
CO₂ (0-15 vol%)

IR
CO₂ (0-1000 ppmv)

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