Uncertainty Analysis for the Parameterization of Glycols

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A review of the 4C association scheme for mono-ethylene glycol (MEG)

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Background

• Collaboration between DTU-CERE and StatOil ASA
• Natural gas dehydration: StatOil Subsea Factory\(^{TM}\) and Gas-2-Pipe\(^{TM}\)
• Important Sales Gas specifications:
  - Hydrocarbon dew point: cricondenbar 105-110 bar
  - H\(_2\)O dew point: 32 ppm
  - Glycol in the gas phase 8 l/MSm\(^3\)

Results and Discussion

Use of pure component experimental data versus pseudo data

• Accuracy of MEG liquid density prediction sacrificed by incorporating the LLE criterion
• MEG vapour pressure data exhibits significantly higher variance than the DIPPR correlation suggests
• Bootstrapped parameter plots show high degree of correlation when fitting to DIPPR

Uncertainty analysis: new CPA-4C MEG parameters

• Literature parameters do not match well with bootstrapped mean parameter estimator
• Mean of the average absolute error and 95% confidence interval over 1500 optimization runs:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Literature</th>
<th>Mean of abs. error</th>
<th>95% CI (lb)</th>
<th>95% CI (ub)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \beta )</td>
<td>1.96</td>
<td>2.01</td>
<td>1.93</td>
<td>2.08</td>
</tr>
<tr>
<td>( \epsilon )</td>
<td>1.27</td>
<td>1.38</td>
<td>1.25</td>
<td>1.41</td>
</tr>
<tr>
<td>( \alpha )</td>
<td>1.13</td>
<td>1.18</td>
<td>1.10</td>
<td>1.26</td>
</tr>
<tr>
<td>( k_{ij} )</td>
<td>1.78</td>
<td>1.96</td>
<td>1.74</td>
<td>2.22</td>
</tr>
</tbody>
</table>

Application for Simplified NG Dehydration Systems

Binary systems

• Improved correlation of the MEG entrained into \( \text{CH}_4 \) rich phase
• Prediction is best at both high temperature and high pressure
• Low temperature anomalies may be due to experimental difficulties

Ternary systems

• Prediction for MEG entrainment is much improved
• \( \text{CH}_4 \) solubility in the liquid phase is underpredicted

Methodology

Parameter evaluation and uncertainty analysis

1. Data selection: pure and multicomponent
2. Determine objective function for parameter estimation:

\[
\text{OF}_{\text{min}}(a_i, b_i, c_i, \epsilon, \beta, k_{ij}) = \sum_i \left( T_{\text{exp}} - T_{\text{cal}} \right) \left( 1 + \frac{1}{\epsilon} - 1 \right) \]

3. Run optimization to obtain new parameters
4. Bootstrap: randomly sample (with replacement) from experimental data and refit parameters according to \( \text{OF}_{\text{min}} \)
5. Repeat Step #4 1500 times
6. Determine parameter distributions and confidence intervals
7. Evaluate performance versus literature

Conclusions

• Excess (unnoticed) parameter correlation avoided by using raw experimental data in optimization routines
• New MEG 4C parameters provide improved description for simplified natural gas dehydration applications
• Accurate prediction of all components in all phases remains challenging
• Discrepancies highlight need for further experimental data and model development

Uncertainty analysis utilized in CPA model development

• Bootstrapping recently used\(^{1,2}\) for CPA parameter estimation of \( \text{CO}_2 \)
• Effect of using pseudo data was not specifically evaluated

Literature survey: data for systems of interest

• Binary data are relatively scarce in the open literature and often incongruent
• Single ternary data set (methane-water-MEG) available\(^7\)
• CPA can model both phases (mixture parameters fitted \( \text{CH}_4 \) solubility data only)

Literature

CPA parameterization of glycols

• CPA\(^{13}\) parameter sets\(^6\) for glycols fitted to pure component DIPPR\(^{13}\) correlations, with liquid-liquid equilibrium (LLE) selection criterion

Future Work

• Generation of new experimental data for additional model evaluation
• Apply uncertainty analysis to newly proposed association schemes
• Inclusion of tri-ethylene glycol (TEG) data and modelling
• Modelling of natural gas dehydration in Aspen

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References


Figure 1: Planned workflow for the Subsea Processing Project

Figure 2: Selected parameter distribution (left) and correlation plots (right), showing confidence intervals developed from the bootstrap method

Figure 3: Correlation of MEG vapour phase fraction in \( \text{CH}_4 \)

Figure 4: Ternary VLE predictions for MEG-\( \text{H}_2\text{O}-\text{CH}_4 \) at 278K and 298K

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