Uncertainty Analysis for the Parameterization of Glycols

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Uncertainty Analysis of the Parameterization of Glycols

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

François Kruger

Supervised by: Nicolas von Solms & Georgios Kontogeorgis

Background

- Collaboration between DTU-CERE and Statoil ASA
- Natural gas dehydration: StatOil Subsea Factory™ and Gas-2-Pipe™
- Important Sales Gas specifications:
  - Hydrocarbon dew point: cricondenbar 105-110 bar
  - H₂O dew point: 32 ppm
  - Glycol in the gas phase 8 l/Sm³

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>Literature</th>
<th>Mean</th>
<th>std</th>
<th>min</th>
<th>5% CI</th>
<th>95% CI</th>
<th>1% CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Literature</td>
<td>51.40</td>
<td>2532</td>
<td>0.6744</td>
<td>2376</td>
<td>14.10</td>
<td>-0.105</td>
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<td>New MEG 4C</td>
<td>1.78</td>
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<td>3.01</td>
<td>4.55</td>
<td>15.4</td>
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Application for Simplified NG Dehydration Systems

Binary systems
- Improved correlation of the MEG entrained into CH₄ 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
- CH₄ solubility in the liquid phase is underpredicted

Conclusions

- 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

Future Work

- Planned workflow for the Subsea Processing Project

Acknowledgement

The authors wish to thank Statoil for their financial support of this research, which is part of the CHIGP (Chemical in Gas Processing) project

Literature Review

CPA parameterization of glycols
- CPA⁴ parameter sets⁵ for glycols fitted to pure component DIPPR⁶ correlations, with liquid-liquid equilibrium (LLE) selection criterion

Uncertainty analysis utilized in CPA model development
- Bootstrapping recently used⁷ to for CPA parameter estimation of CO₂
- 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) available⁸
- CPA can model both phases (mixture parameters fitted CH₄ solubility data only)

Methodology

Parameter evaluation and uncertainty analysis
1. Data selection: pure and multicomponent
2. Determine objective function for parameter estimation:
   \[ \text{OF}_{\text{min}}(a_0, b_0, c_1, \epsilon, \beta, k_{ij}) = \sum \left( t_{\text{calc}} - t_{\text{exp}} \right)^2 \]
   \[ i \in \{ P_{\text{sat}}, \rho, T_{\text{Px}}, T_{\text{Py}} \} \]
3. Run optimization to obtain new parameters
4. Bootstrap: randomly sample (with replacement) from experimental data and refit parameters according to OF_{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

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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 CH₄

Figure 4: Ternary VLE predictions for MEG-H₂O-CH₄ at 278K and 298K

Table 1: Parameter confidence intervals and fitting errors for newly proposed MEG 4C parameters

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