Uncertainty Analysis for the Parameterization of Glycols

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Citation (APA):
Uncertainty Analysis for the Parameterization of Glycols: 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™ 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 improved 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>4C MEG parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid</td>
<td>±0.1</td>
<td>±0.086</td>
</tr>
<tr>
<td>Vapour</td>
<td>±0.1</td>
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</tr>
<tr>
<td>Overall</td>
<td>±0.1</td>
<td>±0.086</td>
</tr>
</tbody>
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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

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

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

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.

Methodology

Parameter evaluation and uncertainty analysis

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

\[ OF_{\text{min}}(a_i, b_i, c_i, \varepsilon, \beta, k_i) = \sum_i \left| \frac{t_{\text{calc}} - t_{\text{exp}}}{t_{\text{exp}}} \right| \]

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

Literature Review

CPA parameterization of glycols

- CPA<sup>2</sup> parameter sets<sup>6</sup> for glycols fitted to pure component DIPPR<sup>3</sup> correlations, with liquid-liquid equilibrium (LLE) selection criterion

Uncertainty analysis utilized in CPA model development

- Bootstrapping recently used<sup>6</sup> 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) available<sup>7</sup>
- CPA can model both phases (mixture parameters fitted CH₄ solubility data only)

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

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References:

- 2. Brigham Young University (BYU).
- 6. Control and subsea processing: New MEG 4C parameters provide improved description for simplified natural gas dehydration applications
- 7. Control and subsea processing: New MEG 4C parameters provide improved description for simplified natural gas dehydration applications
- 8. Control and subsea processing: New MEG 4C parameters provide improved description for simplified natural gas dehydration applications