Uncertainty Analysis for the Parameterization of Glycols

Kruger, Francois

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Uncertainty Analysis for the Parameterization of Glycols
A review of the 4C association scheme for mono-ethylene glycol (MEG)
Francois 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/MSm³

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</th>
<th>95% CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>k₁₂</td>
<td>51.40</td>
<td>0.81</td>
<td>3.01</td>
</tr>
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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

Literature Review
CPA parameterization of glycols

Uncertainty analysis utilized in CPA model development
- Bootstrapping recently used [10] to fit 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 [7]
- 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:

   \[ OF_{\text{min}}(a_i, b_i, c_i, \beta, \kappa_i) = \min \left( \sum (t_{\text{exp}} - t_{\text{fit}}) \right) \]

   \[ i \in \{ \text{Sat}, \rho, \text{TPx}, \text{TPy} \} \]

3. Run 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

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