Uncertainty Analysis for the Parameterization of Glycols

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Uncertainty Analysis of the Parameterization of Glycolysis
A review of the 4C association scheme for mono-ethylene glycol (MEG)
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Background
- Collaboration between DTU-CERE and Statol ASA
- Natural gas dehydration: Statoll Subsea Factory\textsuperscript{(1)} and Gas-2-Pipe\textsuperscript{(2)}
- Important Sales Gas specifications:
  - Hydrocarbon dew point: cricondenbar 105-110 bar
  - H\textsubscript{2}O dew point: 32 ppm
  - Glycol in the gas phase 8 l/MSm\textsuperscript{3}

Phase equilibria measurements and thermodynamic modelling of petroleum fluids relevant to subsea processing

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>95% CI (lb)*</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.6819</td>
<td>14.10</td>
<td>-0.105</td>
</tr>
<tr>
<td>0.6744</td>
<td>23.76</td>
<td>1.96</td>
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<td>0.81</td>
<td>3.01</td>
<td>2.44</td>
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<tr>
<td>4.55</td>
<td>15.4</td>
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</tbody>
</table>

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
CPE parameterization of glycols
- CPA\textsuperscript{(3)} parameter sets\textsuperscript{(4)} for glycols fitted to pure component DIPPR\textsuperscript{(5)} correlations, with liquid-liquid equilibrium (LLE) selection criterion

Uncertainty analysis utilized in CPA model development
- Bootstrapping recently used\textsuperscript{(6)} for CPA parameter estimation of CO\textsubscript{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\textsuperscript{(7)}
- CPA can model both phases (mixture parameters fitted CH\textsubscript{4} solubility data only)

Methodology
Parameter evaluation and uncertainty analysis
1. Data selection: pure and multicomponent
2. Determine objective function for parameter estimation:
   \[ \text{OF}_{\text{min}}(a_i, b_i, c_i, E, \beta, k_i) = \sum \frac{l_{\exp i} - l_{\text{calc i}}}{l_{\exp i}} \]
   \[ i \in \{P_{\text{sat}}, \rho, \text{TPx}, \text{TPy}\} \]
3. Run optimization to obtain new parameters
4. Bootstrap: randomly sample (with replacement) from experimental data and refit parameters according to \( \text{OF}_{\text{min}} \)
5. Repeat Step #4 1500 times
6. Determine parameter distributions and confidence intervals
7. Evaluate performance versus literature

Applications for Simplified NG Dehydration Systems
Binary systems
- Improved correlation of the MEG entrained into CH\textsubscript{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
- CH\textsubscript{4} solubility in the liquid phase is underpredicted

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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CERE
Center for Energy Resources Engineering