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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: Statol Subsea FactoryTM and Gas-2-PipeTM
• 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>Parameter</th>
<th>Literature</th>
<th>Calculation</th>
<th>1500 Data</th>
<th>Bootstrap Mean</th>
<th>95% CI</th>
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<td>2.44</td>
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<td>3.01</td>
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</tbody>
</table>

Literature Review

CPA parameterization of glycols

• CPA9(8) parameter sets9(8) for glycols fitted to pure component DIPPR9(8) correlations, with liquid-liquid equilibria (LLE) selection criterion

Uncertainty analysis utilized in CPA model development

• Bootstrapping recently used10(10) 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) available7(7)
• CPA can model both phases (mixture parameters fitted CH3 solubility data only)

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

• Collaboration between Statoil and DTU-CERE
• Natural gas dehydration: Statol Subsea FactoryTM and Gas-2-PipeTM
• Important Sales Gas specifications:
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