Uncertainty Analysis for the Parameterization of Glycols

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Uncertainty Analysis for the Parameterization of Glycrols

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 FactoryTM(1) and Gas-2-PipeTM(2)
- Important Sales Gas specifications:
  - Hydrocarbon dew point: cricondenbar 105-110 bar
  - H2O dew point: 32 ppm
  - Glycol in the gas phase 8 lMSc-3

- Generation of new experimental data for additional model evaluation
- Liquid phase β point recently
- Collaboration to cricondenbar 2.44 β10
- ASA Inclusion of tri

- Accurate prediction of all components in all phases remains challenging
- Bootstrap: randomly sample (with replacement) from experimental data and
- Bootstrapping parameters
- Density
- DTU often
- phases
- 2376 interval confidence available
- solubility in the liquid
- 2827 data
- 0.6819 Gas
- with thermodynamic
- Factory
- Prediction is best at both high
- CPA parameterization of glycols
- 14.10 Parameter Data fit error [% ARD]
- 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 CH2 solubility data only)

- Parameter evaluation and uncertainty analysis
  1. Data selection: pure and multicomponent
  2. Determine objective function for parameter estimation:
     \[ OF_{\text{min}}(\alpha_i, \beta_i, \epsilon_i, R_i) = \sum |\text{calc} - \text{exp}|/\text{exp} \]
  3. Run optimization to obtain new parameters
  4. Bootstrap: randomly sample with (replacement) from experimental data and
  refit parameters according to \( OF_{\text{in}} \)
  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

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

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

References:

1. Brigham Young University (BYU).
5. Ethylene glycol (MEG)
6. GPAO
7. Literature survey: data for systems of interest

Methodology

- Accuracy ppm and evaluated Mean solubility of the experimental data with Effect DIPPR data
- 
- New considerations for MEG within the association framework e.g. new parameter sets, kij and association schemes

Literature Review

- CPA parameterization of glycrols
- CPAi parameter sets for glycols fitted to pure component DIPPR correlations, with liquid-liquid equilibrium (LLE) selection criterion
- Bootstrapping recently used(6) to for CPA parameter estimation of CO2
- Effect of using pseudo data was not specifically evaluated

- 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

Application for Simplified NG Dehydration Systems

- Ternary systems
- Prediction for MEG entrainment is much improved
- CH4 solubility in the liquid phase is underpredicted

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

Use of pure component experimental data versus pseudo data

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| Parameter confidence intervals and fitting errors for newly proposed MEG 4C parameters |
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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

Technical University of Denmark

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