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Uncertainty Analysis for the Parameterization of Glyceraldehyde

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 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 parameter sets do not match well with bootstrapped mean parameter estimator
- Mean of the average absolute error and 95% confidence interval over 1500 optimization runs:

| Parameter | Literature | 95% CI (lb)* | 95% CI (ub)* | New Data*
|-----------|------------|-------------|-------------|-----------
| ε/R [K]   | 51.40      | 2532        | 0.6744      | 2376       |
| PSat      | 14.10      | -0.105      | 1.96        | 2.44       |
| TPy13     | 4.80       | 2.44        | 4.80        | 4.80       |
| TPx13     | 15.40      | 1.96        | 2.44        | 4.80       |

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

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