# Evaluating CPA equation of state predictive capacities: A study on the transferability of the hydroxyl group associative parameters

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## Supplementary Data

Table A1– Deviations for the calculated pure compound Cp.

| Compound | T range (K) | %AAD Cp |
|---|---|---|
| MEG set 1 | 330-490 | 4.95 |
| MEG set 2 | 330-490 | 4.92 |
| MEG Yeh et al. | 330-490 | 1.34 |
| 1,3-propanediol | 293-353 | 2.20 |
| 1,4-butanediol | 293-353 | 7.77 |
| 1,5-pentanediol | 293-353 | 4.63 |
| 1,5-pentanediol[a] | 358-586 | 1.15 |
| 1,6-hexanediol | 319-353 | 2.67 |
| Glycerol | 330-530 | 15.31 |
| 2-propanol | 293-433 | 1.69 |
| 2-butanol | 254-354 | 1.14 |
| 2-pentanol | 251-361 | 3.99 |
| tert-butanol | 254-424 | 4.82 |

a- 1,5-pentanediol results when compared with the correlation from Rowley et al.

Table A2– Deviations for the VLE at constant pressure.

| Components | %AAD | | | |
|---|---|---|---|---|
| | Bubble temperatures | $y_1$ | Dew temperatures | $x_1$ |
| MEG + ethanol | 0.16 | 1.38 | 0.68 | 0.43 |
| MEG + 2-propanol | 0.41 | 0.59 | 0.81 | 18.15 |
| MEG + 1,3-propanediol | 0.18 | - | - | - |
| MEG + 1,4-butanediol | 0.31 | 4.35 | 0.37 | 6.77 |
| 2-propanol + 1,3-propanediol | 0.48 | 0.72 | 0.08 | 10.60 |
| ethanol + tert-butanol | 0.01 | 0.36 | 0.01 | 0.34 |
| glycerol + methanol | 0.30 | - | - | - |
| glycerol + ethanol | 2.05 | - | - | - |
| glycerol + 1-propanol | 1.47 | - | - | - |
| glycerol + 2-propanol | 1.31 | - | - | - |
| glycerol + 1-butanol | 0.50 | - | - | - |

Table A3– Deviations for the VLE at constant temperature/composition.

| Components | %AAD | | | |
|---|---|---|---|---|
| | Bubble pressures | $y_1$ | Dew pressures | $x_1$ |
| tert-butanol + butane | 4.44 | - | 1.47 | - |
| tert-butanol + isobutylene | 2.17 | 3.20 | 1.67 | 3.82 |
| glycerol + 1,3-propanediol | 19.52 | - | - | - |

Table A4– Comparison between the binary results for MEG + alkanes using the estimated $k_{ij}$ and the correlated $k_{ij}$.

| Component (HC) | %AAD | | | |
|---|---|---|---|---|
| | Solubility of MEG in HC | | Solubility of HC in MEG | |
| | original kij | correlated kij | original kij | correlated kij |
| methane | 46.62 | 45.35 | 3.65 | 5.34 |
| ethane | - | - | 3.64 | 7.86 |
| propane | - | - | 2.57 | 5.94 |
| hexane | 22.35 | 15.95 | 21.72 | 41.45 |
| heptane | 7.07 | 16.02 | 5.40 | 38.30 |
| nonane | 34.45 | 42.78 | 6.75 | 21.93 |

Table A5– Deviations for the remaining LLE and GLE.

| Component 2 | %AAD | |
|---|---|---|
| | MEG rich phase | Component 2 rich phase |
| MCH | 8.33 | 15.29 |
| $CO_2$ | 9.57 | 27.23 |
| $N_2$ | 3.76 | - |
| COS | 6.91 | - |
| $H_2S$ | 12.66 | - |