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Activity Coefficients from Vapor-Liquid Interfaces: A Molecular Dynamics Approach for Separation Chemistry

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Context

- Understanding solvent extraction – Recyclage of rare earth elements and spent nuclear fuels
- Hydrated ions in the aqueous phase
- Extractant aggregates in the organic phase

Methods and concepts

- Measuring activity and the vapor pressure
  - Solvent flow: Vapor pressure of the pure solvent always higher than of a mixtures
  - Ideal case: Solvent vapor pressure by Raoult’s law
  - Otherwise: Aggregation increases, dissolution decreases solvent vapor pressure and thus activity

Aqueous dysprosium nitrate Dy(NO\textsubscript{3})\textsubscript{3} solutions (2)

- Water activity \(a_W\)
- Osmotic coefficient \(\phi_W\)
- Activity coefficient \(Y_E\)

Organic phases – Binary Mixtures of DMDOHHEMA and \(n\)-heptane

- Molecular dynamics simulation of liquid-vapor equilibria of organic solvent phases containing:
  - Pure solvent + Extractant + Water + Ionic species
  - Aggregation of DMDOHHEMA in the organic phase relies on the availability of water\textsuperscript{29}

Outlook and conclusion

- Aqueous salt solutions: Results from molecular dynamics simulation are in good agreement with experimental data for different nitrate salts. This approach can be used for the validation of force fields for MD simulation with respect to thermodynamic properties.
- Organic Phases: Method has been successfully applied on binary mixtures (\(n\)-heptane and DMDOHHEMA, but also ethanol and water\textsuperscript{16}). Allows accessing more complex organic solvent phases containing water and ionic species.
- Simulation of activity coefficients of complex solutions with volatile solvents for understanding solvent extraction

References


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