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

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\(p_2\): Vapor pressure of pure solvent

**Methods and concepts**

- **Hydrated ions in the aqueous phase**
- **Extractant aggregates in the organic phase**
- **Aqueous electrolyte solution**
- **Organic solvent phase**

**Context**

- Understanding solvent extraction – Recycling of rare earth elements and spent nuclear fuels
- Ideal case: Solvent vapor pressure
- Molecular dynamics
- 1982
- Controlling the error of the method
- Exchange
- The error of the method
- Vapor
- of
- The liquid
- Simulation of activity coefficients of
- Marcoule
- Vapor
- A
- (SPDS/LILA), BP 17171, F
- Solvent flow
- Activity coefficient
- Attractive and repulsive interactions in the mixtures cancel out
- computing
- Organic Phases:
- and
- possible
- the
- Montpellier
- Meridiano,
- O
- made
- 2017
- Rard
- Extr
- concentration
- high
- (5
- and DMDOHEMA show ideal behavior
- Otherwise:
- relation
- Processes
- Aqueous salt solutions:
- law
- Molecular Dynamics using
- Aggregation of DMDOHEMA in the
- Equilibria
- in Marcoule (ICSM, CEA
- 2018
- Michaelbley@outlook.com
- michael.bley@cea.fr

**Aqueous dysprosium nitrate \(\text{Dy(NO}_3)_3\) solutions**

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

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

- Molecular dynamics simulation of liquid-vapor equilibria of organic solvent phases containing:
- Pure solvent
- Extractant
- Water
- Ionic species
- Increasing computational cost
- Aggregation of DMDOHEMA in the organic phase relies on the availability of water
- \(\lambda\): Time of flight
- \(\sigma_0(t)\): Relative error of the method
- \(a_{SOL}\): Solvent activity

**References**


**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 DMDOHEMA, but also ethanol and water): 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**

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