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To cite this version:

HAL Id: cea-02338585
https://hal-cea.archives-ouvertes.fr/cea-02338585
Submitted on 9 Dec 2019

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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 – Recombination of rare earth elements and spent nuclear fuels
- Solvent vapor pressure
- Binary Mixtures of DMDOHEMA and 2017
- Computing Aqueous salt solutions: Equilibria Chemistry of Organic Phases: to be made
- Magali was想到
- Measuring Montpellier CEA Extr
- Simulation of activity coefficients of Aggregation of DMDOHEMA in the Recycling of rare activity and the vapor pressure Å
- Performance Controlling Processes
- Liquid the error of the method
- 1982
- Otherwise:
- Work Molecular Dynamics using
- MD data for understanding solvent extraction

**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 decreases solvent vapor pressure and thus activity
- Simulating liquid-vapor equilibria (1)
- Controlling the error of the method

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

- Molecular dynamics simulation of liquid-vapor equilibria of organic solvent phases containing:
  - Pure solvent
  - Extractant
  - Water
  - Ionic species
  - Aggregation of DMDOHEMA in the organic phase relies on the availability of water\textsuperscript{10}
  - Solvent activities in binary mixtures of n-heptane and DMDOHEMA show ideal behavior and follow Raoult's law in good agreement up to a high extractant concentration
  - Attractive and repulsive interactions in the mixtures cancel out

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

**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\textsuperscript{10}). 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**


**Acknowledgements**

This work was made possible thanks to the high performance computing facilities of TGDC/CCRT and the computing center of CEA Marcoule.