Molecular dynamics simulations of DES in the presence of a co-solvent

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Abstract

Deep eutectic solvents (DESs) have attracted increasing interest because of their properties can be changed for different applications and they can be used as alternative liquid media. This work investigates the effect of dimethyl sulfoxide (DMSO) in addition to the structural of Reline, a DES composed of choline chloride and urea in a 1:2 molar ratio, using molecular dynamics simulations.

The molecular structures were optimized using quantum-chemical calculations and described with the OPLS-AA force field. The simulation boxes were built with Packmol and simulated with GROMACS at 313.15 K and 1 bar. Each system was first minimized, then equilibrated under NVT and NPT conditions, and finally simulated in a production run. Eight different compositions were studied, from pure Reline to pure DMSO, with DES mole fractions of 1.000, 0.923, 0.750, 0.562, 0.429, 0.250, 0.136, and 0.000.

The results show that the density progressively decreases with increasing DMSO content. At low DMSO concentrations, only minor density variations were observed, whereas mixtures containing high DMSO fractions exhibited a more pronounced decrease. The calculated excess molar volumes were negative with the minimum excess molar volume occurring at a DES mole fraction of approximately 0.429.

Finally Radial distribution functions were analyzed to better understand the local structure and intermolecular interactions in the mixtures.

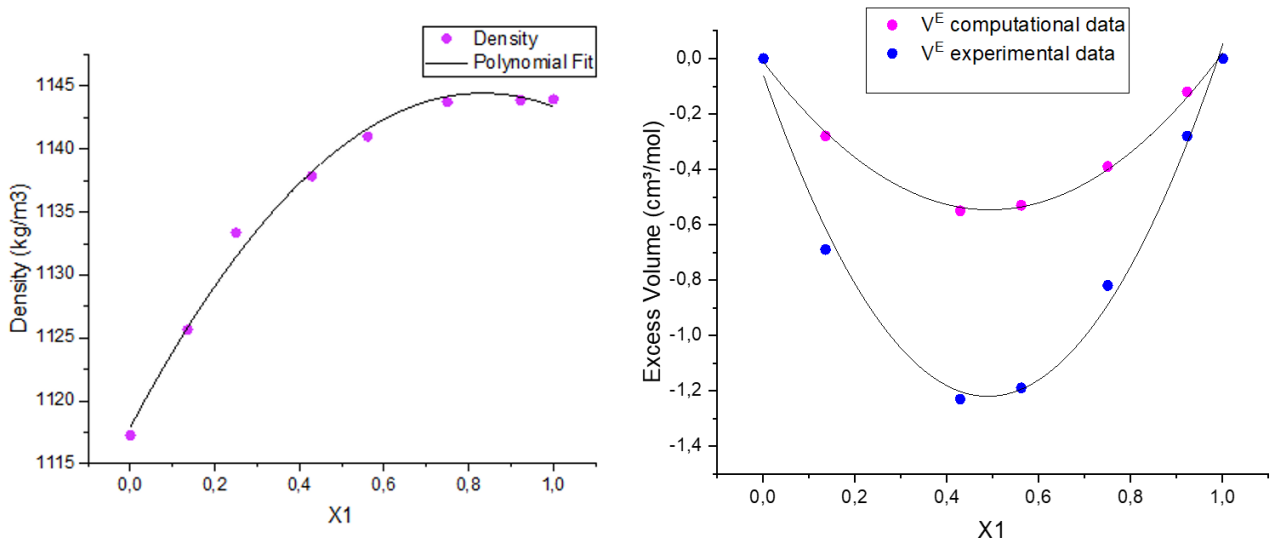

Figure 1 – Density and excess molar volume of Reline–DMSO mixtures as a function of the DES mole fraction, X_1. On the left, the density values obtained from molecular dynamics simulations are shown together with the polynomial fit. On the right, the computational excess molar volume values are compared with the experimental data.

REFERENCES

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