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Influence of electrolytes on liquid-liquid equilibria of water/1-butanol and on the partitioning of 5-hydroxymethylfurfural in water/1-butanol

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Abstract

The influence of electrolytes on liquid-liquid equilibria (LLE) of water/1-butanol and on the partitioning of 5-hydroxymethylfurfural (HMF) between water-rich and 1-butanol-rich phases was investigated in this study. For that purpose, the LLE of the ternary systems water/1-butanol/HMF, water/1-butanol/salt, and the LLE of the quaternary system water/1-butanol/HMF/salt were measured at 298.15 K under atmospheric pressure. The investigated salts were composed of one of the anions Cl^- , CH_3COO^- , NO_3^- and SO_4^{2-} and either Li^+ or Na^+ . By investigating the LLE of the system water/1-butanol/salt it was found that 1-butanol was salted-out from the aqueous phase by all salts, and the strength of the salting-out increased in the following order $\text{NO}_3^- < \text{CH}_3\text{COO}^- \approx \text{Cl}^- < \text{SO}_4^{2-}$, independently of the cation.

Based on the LLE data, the partition coefficient $K_{\text{HMF}}^{\text{W}}$ of HMF between 1-butanol and aqueous phase was determined. Li_2SO_4 caused a pronounced salting-out of HMF from the aqueous phase, whereas only a moderate influence was observed for NaCl and CH_3COONa . LiCl even caused a salting-in at LiCl molalities above 6 mol/kg_{H₂O}. electrolyte Perturbed-Chain Statistical Associating Fluid Theory (ePC-SAFT) was successfully used to model the influence of salts on the LLE water/1-butanol. Without fitting parameters to LLE data of the quaternary system water/1-butanol/HMF/salt, ePC-SAFT allowed predicting the salt influence on the partitioning of HMF in these systems in good agreement with the experimental data.

Keywords: HMF, LLE, salt, ePC-SAFT, salting-out, extraction, prediction, modeling

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