Molecular Kinetic Extraction Mechanism Analysis of 1-butanol from N-heptane-1-butanol by Choline-based DESs as Extractants

Deep eutectic solvent (DES) is considered as a new generation of green solvent due to its advantages such as simple preparation, low price and easy to degrade. In this work, the extraction mechanism of 1-butanol separation from alkanol azeotropic system using choline-based DES was studied. The extraction process was repeated by molecular dynamics(MD) simulation. According to MD simulation results, the nonbonded interaction energies, radial distribution functions, spatial distribution functions and self-diffusion coefficient between different DES and different components were calculated and compared. The results showed that ChCl (choline chloride)/urea (1:2) was one of the four DESs with the best extraction effect, which was very consistent with the experimental results. Through the further analysis of the simulation results, it was found that the hydrogen bond donor in DES had great influence on its extraction efficiency. For the same kind of DES, anion played a dominant role in the extraction of 1-butanol. This work provided some theoretical guidance for the recovery of 1-butanol and the use of choline-based DES, and supplied some reference for the screening of DES.