577b Molecular Dynamics Study of Propanic Acids at the Water-Isobutanol Interfaces

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The enhancement of interphase mass transfer is a key issue in liquid-vapor absorption systems and in liquid-liquid extraction systems. The study of the partition of propanoic acid between water and isobutanol may be interesting for industrial applications, because organic acids in aqueous solutions are diluted by extraction with alcohols. Besides, in this system the interfacial turbulence occurs when the acid transfers from isobutanol to water and from water to isobutanol though the theory of Sterling and Scriven predicts that the interfacial turbulence occurs only when the acid transfers from isobutanol to water [1]. In the present study, molecular dynamics simulations were used to clarify (a) the distribution of propanic acids at the water-isobutanol interfaces and (b) the mechanism and conditions involved in the generation of fluctuations that lead to interfacial turbulence.

The calculation system and methodology are the same to the previous molecular dynamics study of n-alcohols adsorbed on an aqueous electrolyte solution [2]. In the previous study, the stability of the alcohol distribution was studied for three types of n-alcohol (n-propanol, C3H7OH; n-heptanol, C7H15OH; and n-undecanol, C11H23OH), various concentrations of alcohol. The simulation results reveal that the distribution of n-propanol on water is homogeneous at all n-alcohol concentrations and the distribution of n-heptanol and n-undecanol on water is heterogeneous. The n-alcohol concentration at which fluctuations in the alcohol distribution begin to increase depends on the length of the hydrocarbon chain of the n-alcohol. In the present study, the calculation results of the density and the local surface tension profiles along the direction normal to the interface show that as the concentration of propanic acid increases, the interface region increases and the surface tension decrease continuously. But when the concentration of propanic acid is over a critical value, water, isobutanol and propanic acid mix well. The details of the structural and dynamical properties of propanic acid at the interface were discussed.

References [1] M. Vanni and G. Baldi, Trans. IchemE 71A (1993) 119-126. [2] H. Daiguji, J. Chem. Phys. 115 (2001) 1538-1549.