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Separation of 2,4,6-Trinitrophenol from Aqueous Solution by Liquid-Liquid Extraction Method : Equilibrium, Kinetics, Thermodynamics and Molecular Dynamic Simulation

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ABSTRACT

In this paper, the equilibrium and kinetic studies on the extraction of 2,4,6-Trinitrophenol (picric acid) (0.021 - 0.061 kmol·m^{-3}) using Amberlite LA2, a secondary amine (ALA2: 0.118 - 0.588 kmol·m^{-3}) dissolved in a polar active solvent, methyl-iso-butyl ketone (MIBK) are performed. Also, the temperature effect (293.2 ± 1 K, 303.2 ± 1 K and 313.2 ± 1 K) on the extraction mechanism and efficiency is evaluated. Thermodynamic parameters like the change in entropy and enthalpy are determined. From the values of loading ratio ($Z < 0.5$), it is inferred that the amine molecule form 1:1 complex with the acid molecule in the organic phase. The mass transfer coefficient (k_L = 3.1×10^{-5} m·s^{-1}) of picric acid in MIBK is determined. The *Hatta* number is calculated, and observed to vary in the range of 0.0032 to 0.0054, indicating that there is a very slow chemical reaction taking place between the acid and the amine molecule in the bulk of the organic phase. The reaction order is estimated to be 0.9 w.r.t picric acid, and 0.6 w.r.t ALA2 with rate constants of 14.95 × 10^{-6} (kmol·m^{-3})$^{-0.5}$s^{-1}, and 8.94 × 10^{-7} (kmol·m^{-3})$^{-0.5}$s^{-1}, for forward and backward reaction, respectively. Kinetic and potential energies of components during reactive extraction have been determined by molecular dynamic modeling.

Keywords: Picric acid; extraction; equilibrium; kinetics; thermodynamics; molecular modeling.