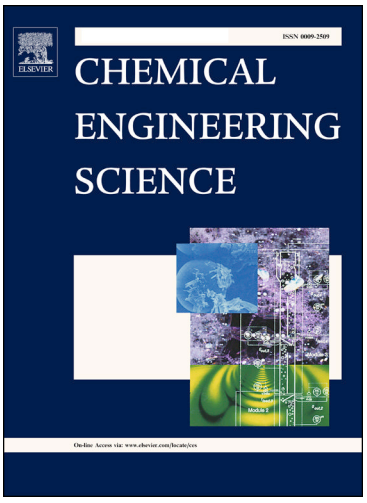

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Screening of Imidazolium Ionic Liquids for the Isobutane Alkylation Based on Molecular Dynamic Simulation

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ABSTRACT: In the liquid/liquid reaction of isobutane alkylation with C4 olefin, the solubility and diffusion properties of isobutane in catalyst phase exert substantial effect on the quality of alkylate. The solubility, diffusion, and permeability of isobutane and 2-butene in the 1-alkyl-3-methylimidazolium ionic liquids (ILs) with various anions including [BMIm][PF_6], [BMIm][BF_4], [BMIm][Tf_2N] and [BMIm][Al_2Cl_7], and other ILs with different alkyl chains length including [BMIm][$AlCl_4$], [HMIm][$AlCl_4$] and [OMIm][$AlCl_4$], as well as the H_2SO_4, were investigated using molecular dynamic simulation. Compared to H_2SO_4, the ILs were more favorable for the dissolution and diffusion of isobutane. The predicted isobutane solubility in ILs follows the order of [BMIm][Al_2Cl_7]> [BMIm][$AlCl_4$]> [BMIm][Tf_2N]> [BMIm][PF_6]> [BMIm][BF_4] for ILs with different anions, and [OMIm][$AlCl_4$]> [HMIm][$AlCl_4$]> [BMIm][$AlCl_4$] for ILs with different alkyl chain length. The higher solubility of isobutane can be ascribed to the weaker cation-anion interaction, lower solubility parameter, and larger free volume. The isobutane diffusion follows the same trend as solubility for ILs with different anions, but

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