Predicting the Solubility of Aromatic Waste Petroleum Paraffin Wax in Organic Solvents to Separate Ultra-Pure Phase Change Materials (PCMs) by Molecular Dynamics Simulation

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Abstract : With the ultimate goal of developing the separation of n-paraffin as phase change material (PCM) by means of molecular dynamic simulations, we attempt to predict the solubility of aromatic n-paraffin in two organic solvents: Butyl Acetate (BA) and Methyl Iso Butyl Ketone (MIBK). A simple model of aromatic paraffin: 2-hexadecylantharacene with amorphous molecular structure and periodic boundary conditions was constructed. The results showed that MIBK is the best solvent to separate ultra-pure phase change materials and this data was compatible with experimental data done to separate ultra-pure n-paraffin from waste petroleum aromatic paraffin wax, the separated n-paraffin was characterized by XRD, TGA, GC and DSC, moreover; data revealed that the n-paraffin separated by using MIBK is better as PCM than that separated using BA.

Keywords : molecular dynamics simulation, n-paraffin, organic solvents, phase change materials, solvent extraction
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