Journal Article – Volume 149, Issue 17, Journal of Thermal Analysis and Calorimetry 2020, Pages 9203 - 9221

Microscopic molecular insights of different carbon chain fatty acids on shape-stabilized phase change composite

Abstract

Biochar-based composite phase change materials (PCMs) are gaining popularity in thermal energy storage (TES) applications. Organic PCMs derived from fatty acids are favored for their affordability and variable melting temperatures based on carbon chain length. Understanding the interaction between different carbon-length fatty acid PCMs and porous biochar is crucial for optimizing thermal performance. Thus, this study explored the interaction between PCMs of decanoic acid (DA) and octadecanoic acid (OA) with banana peel (BP) biochar. Experimental results showed that shorter carbon chain of DA enhanced thermal properties and surface compactness compared to OA. BP-DA had higher loading efficiency and PCMs ratio, resulting in superior thermal cycle endurance and latent heat ratio. The molecular dynamics suggest that longer carbon chains affect the mean square displacement (MSD) curves, reducing the self-diffusion coefficients of BP-DA. This is due to DA's high loading rate, which occupies more space within BP biochar structure, thus limiting its diffusion capacity. Enhanced hydrogen bonding constrained DA's thermal motion during phase transition, restricting atom mobility within BP. With temperature elevations, BP-DA exhibits lesser fractional free volume than BP-OA, due to lower molecular mass. This research highlights how carbon chain length influences composite PCMs performance, offering insights for efficient TES system design.

Keywords

Carbon chain; Composite; Free volume theory; Mean square displacement; Molecular dynamics; Phase change materials