

Multi-technique investigation on the surface interaction of diatomaceous earth with organic phase change material: Experimental and molecular dynamics aspects

Abstract

To promote diatomaceous earth (DE)-based phase change composite as green energy building materials, this paper bridges the studies of experimental and molecular dynamics (MD) focusing on the absorption effect of phase change materials (PCMs). Octadecanoic acid (OA) was selected as PCMs and DE as supporting material for the fabrication of composite PCMs at different loading ratios; effect on thermal properties and porosity of the composite PCMs were further investigated by MD simulation. In consonance with ATR-FTIR and XRD analyses, the highest loading ratio (DEOA-4) was proven to absorb a high amount of PCMs, with excellent thermal stability and chemical compatibility. DEOA-4 exhibited higher latent heat storage capacity of 52.67 J/g, with a loading ratio and loading efficiency of 32.13 and 32.98 %. Besides, MD simulation showed that increasing the OA loading would decrease the fractional free volume of DEOA models, resulting in a limited mobility of PCMs molecules, as confirmed by self-diffusion coefficient at room and melting temperatures. Experimental and computational studies revealed that pore-filling process plays an imperative role during PCMs absorption. An adequate amount of loading ratio can potentially enhance the pore-filling process, maximize the efficiency of the performances, and promote the development of green energy in concrete structures. © 2023 Elsevier B.V.

Keywords

Diatomaceous earth; Free volume theory; Molecular dynamics; Phase change material; Thermal energy storage