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Molecular Dynamics Simulation of the Effect of the Solid Gas Interface Nanolayer on Enhanced Thermal Conductivity of Copper-CO2 Nanofluid

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Abstract : The use of CO₂ in oil recovery and in CO₂ capture and storage is gaining traction in recent years. These applications involve heat transfer between CO₂ and the base fluid, and hence, there arises a need to improve the thermal conductivity of CO₂ to increase the process efficiency and reduce cost. One way to improve the thermal conductivity is through nanoparticle addition in the base fluid. The nanofluid model in this study consisted of copper (Cu) nanoparticles in varying concentrations with CO₂ as a base fluid. No experimental data are available on thermal conductivity of CO₂ based nanofluid. Molecular dynamics (MD) simulations are an increasingly adopted tool to perform preliminary assessments of nanoparticle (NP) fluid interactions. In this study, the effect of the formation of a nanolayer (or molecular layering) at the gas-solid interface on thermal conductivity is investigated using equilibrium MD simulations by varying NP diameter and keeping the volume fraction (1.413%) of nanofluid constant to check the diameter effect of NP on the nanolayer and thermal conductivity. A dense semi-solid fluid layer was seen to be formed at the NP-gas interface, and the thickness increases with increase in particle diameter, which also moves with the NP Brownian motion. Density distribution has been done to see the effect of nanolayer, and its thickness around the NP. These findings are extremely beneficial, especially to industries employed in oil recovery as increased thermal conductivity of CO₂ will lead to enhanced oil recovery and thermal energy storage.

Keywords : copper-CO2 nanofluid, molecular dynamics simulation, molecular interfacial layer, thermal conductivity
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