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Comprehensive analysis of dispersion and aggregation morphology of nanoparticles on the thermophysical properties of water-based nanofluids using molecular dynamics simulation

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Highlights

- With increasing temperature and SVF, the D_{NF} would increase and decrease, respectively.
- Also, with increasing the SVF and temperature, the μ_{NF} increases and decreases, respectively.
- As the radius of the nanoparticles increases, the D_{NF} increases, and μ_{NF} decreases.
- NFs containing cylindrical nanoparticles have a lower D_{NF} than NFs created by spherical nanoparticles.
- As the SVF, temperature, and radius of the nanoparticles increase, the k_{NF} increases.

Abstract

Background

In recent decades, using nanofluids (NFs) to improve the thermal properties of the NFs was widely considered.

Methods

In the current study, molecular dynamics (MD) simulation was used to examine the effects of dispersion and morphology of nanoparticle aggregation (NA), solid volume fraction (SVF), temperature (Temp), nanoparticle size (NS), and nanoparticle shape on the thermal properties of water/Nickel nanofluid (NF). The thermophysical properties of the NFs were simulated and studied using MD simulation, which was a common computational method because of the high cost and limitations of experimental approaches, particularly at molecular dimensions. LAMMPS software package, and the EAM potential function were used to simulate the structure. In the present simulation, three NF samples containing Ni with SVF of 1, 2, and 3% with two shape of spherical (SN) and cylindrical (CN) and in two different Temp of 313 to 358K were considered. Also, the nanoparticles (NPs) with the radii of 8, 10, and 12Å were considered in the simulation box. The results show that by increasing Temp and SVF, the diffusion coefficient (D_{NF}) of NFs would increase and decrease, respectively. From a numerical point of view, by increasing Temp from 313K to 358 K in 1% SVF, thermal conductivity (k_{NF}) and D_{NF} increased from 0.25456 to 0.33688 W/mK and 0.3478027 to 0.6835048, respectively. Moreover, by increasing SVF and T, the viscosity (μ_{NF}) of NF increased and decreased, respectively.