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Investigation of enhanced thermal properties in NiO-based nanofluids for concentrating solar power applications: A molecular dynamics and experimental analysis

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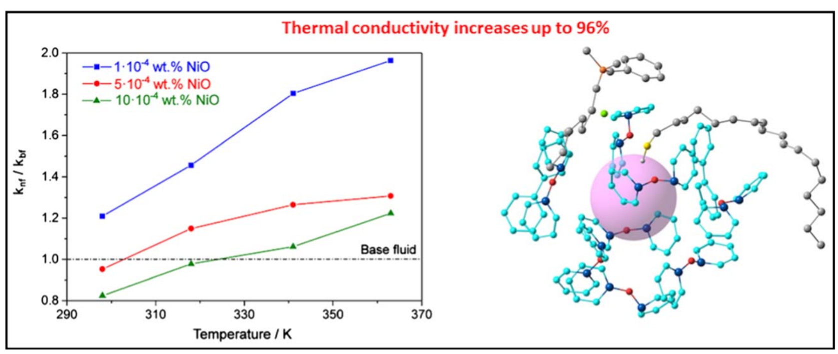
HIGHLIGHTS

- NiO-based nanofluid improves the heat transfer process in Concentrating Solar Power.
- The thermal conductivity was improved up to 96%.
- The heat transfer coefficient was improved by 50%.
- The surfactant plays an important role in the properties of the nanofluid system.
- The arrangement of the base fluid around the nanoparticles is revealed from MD results.

GRAPHICAL ABSTRACT



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ABSTRACT

Nanofluids could be a promising alternative to the typical heat transfer fluids (HTF) used in concentrating solar power. This study analyses nanofluids based on a typical HTF for concentrating solar power (CSP) applications and NiO nanoparticles. The optimum nanoparticle concentration was determined by analysing the stability of the nanofluids. Some of their properties, such as density, viscosity, isobaric specific heat and thermal conductivity, were characterized to evaluate their performance. Their thermal conductivity increased by up to 96% and the heat transfer coefficient by 50%. Molecular dynamics calculations were performed to explain from a molecular perspective how the presence of equal proportions of two surfactants, benzalkonium chloride (BAC) and 1-Octadecanethiol (ODT), enhanced the thermal properties of the NiO nanofluid. The isobaric specific heat and thermal conductivity values followed the same experimental tendency. The analysis of the radial distribution functions (RDFs) and spatial distribution functions (SDFs) revealed an inner layer of base fluid and surfactant molecules around the NiO cell. This first layer contained BAC molecules at all the temperatures, while

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ODT was only incorporated at higher temperatures. The exchange of surfactant and base fluid molecules around the NiO as the temperature increases may play an important role in the enhancement of the thermal properties.

1. Introduction

Concentrating solar power (CSP) is recognised as an interesting source of renewable energy in line with the objective established by society of confronting the growing demand for energy while minimizing environmental harm [1]. The main problem with CSP is its high cost compared with conventional energy sources. For this reason, several lines of research exist that aim to reduce the costs or improve the overall efficiency of CSP plants. One of these involves studying how to enhance the efficiency of the heat transfer processes taking place in the plants by improving the thermal properties of the heat transfer fluid used. In this sense, the use of nanofluids could be an interesting way of improving the thermal properties of the HTF [2–4]. Nanofluids are colloidal suspensions of nanometric particles in a base fluid [5], and the suspension of solids in fluids is known to improve some thermal properties of HTFs, such as its thermal conductivity [3,6–12], isobaric specific heat [3,9,13–16]. Nanofluids can also improve the heat transfer coefficient [16–18]. Recent studies have reported achieving enhanced thermal performance by using nanofluids in solar collectors [19–21]. In addition, the optical properties of nanofluids for use in solar collectors have been studied recently [22–24]. Also, the new system applied in CSP requires a high operating temperature and nanofluids could be a way to increase it [25], and also to improve the thermal storage properties in CSP systems [26]. Thus, nanofluids are a promising alternative that could make CSP plants more efficient and reduce their costs [27].

Therefore, this study presents the preparation of nanofluids based on the eutectic mixture of biphenyl and diphenyl oxide as the base fluid, which is a typical HTF used in CSP plants. NiO nanoparticles were used to prepare the nanofluids because the incorporation of metal oxide nanoparticles is known to increase the thermal conductivity of base fluids [9,12,28]. The stability of the nanofluids was analysed, as were their properties related with their efficiency in the heat transfer process, such as their density, viscosity, isobaric specific heat and thermal conductivity. In addition, the structural properties of the NiO-nanofluid system were obtained by analysing their radial distribution function (RDF) and spatial distribution function (SDF), and how these varied according to temperature. Therefore, the approach based on the analysis of the macroscopic properties of the nanofluids using nano-level interactions is clearly new and original. Moreover, this is the first time that nanofluids based on this base fluid and the use of metal oxide nanoparticles has been studied. The non-polar nature of the base fluid makes it clearly different to other typical base fluids used, such as water or ethylene glycol.

2. Material and methods

2.1. Experimental

The nanofluids analysed in this study were prepared using the two-step method. The first step involves the synthesis of nanoparticles and the second is the dispersion of the nanomaterial into the base fluid. In this study, the base fluid was a commercial heat transfer fluid composed of the eutectic mixture of biphenyl ($C_{12}H_{10}$, 26.5%) and diphenyl oxide ($C_{12}H_{10}O$, 73.5%), supplied by The Dow Chemical Company©, model Dowtherm A. Both compounds show practically the same vapour pressure so the mixture is usually treated as a single compound. The nanomaterial added to the base fluid was commercial NiO nanoparticles (purity ~ 99.8%, density 6670 kg m^{-3} at 298.15 K, Sigma-Aldrich).

An initial colloidal suspension of NiO nanoparticles in the base fluid was prepared with a nominal nanoparticle mass concentration of 0.01 wt.%. A mixture of benzalkonium chloride (BAC, Sigma-Aldrich©) and 1-Octadecanethiol (ODT, purity: 98%, density 0.847 kg m^{-3} at 298 K, Sigma-Aldrich©) was added. The proportion added was 75% of each with regard to the nominal nanoparticle mass concentration. The complete mixture was homogenized for 20 min using a Sonics Vibra Cell VCX 750 sonicator (~50 W output power) in a bath at 288 K. Aliquots of the initial solution were extracted to prepare nanofluids with the nominal NiO nanoparticle mass concentration of $1 \cdot 10^{-4}$; $5 \cdot 10^{-4}$ and $10 \cdot 10^{-4}$ wt.%, adding the base fluid necessary to obtain 100 mL of nanofluid. The new nanofluids underwent sonication under the same conditions as the initial nanofluid. The nanofluids are named using the nominal nanoparticle concentration throughout this article.

The nanofluids were characterised to analyse their stability and performance as heat transfer fluids. Stability is one of the key concepts in colloidal suspensions since their thermal properties depend on it. UV–vis spectroscopy (UV–vis) can provide a measurable characterization of stability by evaluating the absorbance of a suspension [29]. To this end, UV–vis spectra were recorded using an OceanOptics© DH-2000-Bal halogen lamp and an OceanOptics© USB-2000+ monochromator operating in the 400–880 nm wavelength range, using a glass cuvette at room temperature. The sedimentation process can be analysed from particle size measurements. Particle size and size distribution was measured by a Zetasizer Nano ZS using the dynamic light scattering (DLS) principle as a simple method for analysing suspension stability and particle size measurements in solution [28,30]. Also, ζ potential measurements were performed using a Zetasizer Nano ZS supplied by Malvern Instruments Ltd. This system uses the principle of electrophoresis light scattering (ELS), in which charged particles suspended in a fluid are attracted towards the oppositely charged electrode when an electric field is applied. The ζ potential measurements were performed applying a potential of 120 V at 313 K, and the results were analysed using the Huckel model, typical for low dielectric constant fluids.

Density, viscosity, isobaric specific heat and thermal conductivity were determined to characterize the performance of the nanofluids. Density was estimated using a pycnometer and a thermal bath supplied by Select© to control the temperature of the measurements. The density values of each nanofluid were determined five times to obtain the most accurate value. Dynamic viscosity was measured using a SV-10 viscometer supplied by A&D Company Ltd. A water-circulating bath supplied by VWR© with heating and cooling features was used to keep the nanofluids at room temperature during the experiment. The measurements were performed five times to calculate the average values. The isobaric specific heat measurements were performed using a temperature-modulated differential scanning calorimeter (TMDSC), supplied by TA Instruments©, model Q-20. To perform the measurements, a program was created which can be summarized as: the temperature was equilibrated at 341 K to remove contaminants and kept isothermal for 10 min; next, the samples were equilibrated at 301 K and then ramped to 391 K at 1 K/min. A modulation was programmed around the studied temperatures with an amplitude of ± 1 K and a period of 120 s. Finally, cooling was performed at 1 K/min. The isobaric specific heat of the base fluid was measured to compare the method used with the values reported by the supplier. Finally, the thermal conductivity of the nanofluids was measured at several temperatures using the laser flash technique (LFA 1600 equipment, supplied by Linseis Thermal Analysis©). This technique really measures thermal diffusivity, which is the thermophysical property that defines the speed of heat propagation

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