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Towards a multiscale simulation approach of nanofluids for volumetric solar receivers: Assessing inter-particle potential energy

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Abstract

A modern concept for solar thermal collectors is based on volumetric absorption of sunlight, where nanoparticles suspended in liquids directly receive the incident radiation. Suspending nanoparticles in traditional fluids can drastically enhance their optical properties and improve thermo-physical performances, thus leading to highly efficient volumetric solar receivers. Several studies have been addressed on the physical understanding of such nanosuspensions; however, the relation between nanoscale effects and macroscopic properties is far from being fully understood. The present work represents a first step towards a multiscale modelling approach for relating nanoscale properties to macroscopic behaviour of nanofluids. In particular, a suitable Coarse-Grained (CG) method for nanofluids is described. By means of Molecular Dynamics (MD) simulations, the pair Potential of Mean Forces (pPMF) between CG beads of nanofluid is evaluated. A complete CG force field can be then defined by including the effects of water adsorbed at solid-liquid interface, nanoparticle surface charge and solution pH. Our multiscale model is intended to permit a future study of the complex mechanisms of nanoparticle clustering, which is known to affect nanofluids stability and properties. We hope that this multiscale approach may start the process of rational design of nanofluids thus facilitating technology transfer from lab experiments to large-scale industrial production.

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1. Introduction

The majority of current solar thermal technologies exploits absorbing surfaces for converting solar radiation into thermal energy, which is in turn transferred to a carrier fluid by conduction. Such surfaces are designed to have both high absorptivity in the solar spectrum and low emissivity in the infrared. However, the thermal resistance between heat transfer fluid and absorbing surface may induce large temperature differences between fluid and absorber, therefore leading to significant emissive losses and thus reducing the overall solar energy conversion efficiency [1]. These thermal re-radiation losses are particularly evident at high levels of solar concentration, as in Concentrated Solar Power (CSP) plants.

On the other hand, volumetric solar receivers are based on fluids directly absorbing the incident radiation, which leads to decreased temperature differences between absorber and carrier fluid [2]. Nanofluids are engineered suspensions of nanoparticles, which show peculiar optical, heat and mass transport properties in both engineering [3-6] and biomedical applications [7-9]. Because of these characteristics and of the large surface to volume ratio, nanoparticle suspensions have been investigated as solar absorbing fluids for highly efficient volumetric receivers [10, 11]. However, nanofluids are a prototypical example of complex multi-scale systems [12, 13], which makes difficult to relate nanoscale characteristics with resulting macroscopic properties. In particular, the complex mechanism of nanoparticle clustering is known to rule nanofluids stability as well as effective optical and thermal properties [14, 15]. In order to properly take into consideration nanoscale effects in nanofluids, multiscale simulation methods are needed to guide their accurate prediction and rational design in the near future.

Coarse-Grained (CG) is a modelling technique able to bridge Molecular Dynamics (MD) simulations from atomic scale to mesoscale. The basic idea of coarse graining is to combine several atoms into homogeneous groups (CG beads), which interact each other by means of bonded and non-bonded interaction potentials. Numerous coarse-grained techniques have been proposed in the last decades, and they can be classified into top-down or bottom-up methods. In the former, many-body potentials are parameterized in order to reproduce the thermodynamic properties observed at larger scales. For example, Martini Coarse-Grained force field and its further extensions follow the top-down philosophy and are widely used to study complex biomolecular systems [16]. In the bottom-up approach, instead, the effective potentials between CG beads are developed to represent atomistic features. Among the bottom-up techniques, effective CG potentials can be defined by iterative processes, with the aim to reproduce a target radial distribution function [17-19], or force distribution in the atomistic system [20-22]. Although these methods are largely employed and provide accurate descriptions for several physical systems, unphysical CG potentials could result from these optimization approaches. Therefore, some novel CG methods have been recently designed for condensed matter systems. Such non-iterative methods include the pair Potential of Mean Forces (pPMF) [23], the Effective Force Coarse Grained (EFCG) [24] and the Conditional Reversible Work (CRW) [25].

Here, a suitable bottom-up CG model for nanofluids is employed for directly evaluating the pPMF from MD simulations. In particular, a couple of alumina nanoparticles (NPs) solvated in water is chosen as an exemplificative building block for nanofluids for volumetric solar receivers [26]. Preliminary analyses about the interaction energies between the NPs clarify the role of Coulomb and Lennard-Jones potentials in the resulting inter-particle energy.

2. Methods

To evaluate the pPMF between suspended Al_2O_3 nanoparticles (NPs) in water, MD simulations are carried out by using GROMACS package [27]. The following steps describe the adopted simulation protocol ("pulling procedure").

First, the atomistic model of Al_2O_3 NP is prepared by defining the particle geometry and atomistic force field. Specifically, a 2 nm alumina sphere is functionalized by adding OH terminal groups on the surface. All bonds, angles and dihedral within the NP core are modeled with a harmonic potential; instead, Lennard-Jones and Coulomb potentials are imposed for mimicking non-bonded interactions. The CLAYFF force field is adopted for distributing partial charges on the NP surface, which is overall neutral [28].

Second, two alumina nanoparticles are considered. The NPs couple is placed in a box (22x8x8 nm) made of SPC/E water molecules [29]. After the energy minimization, the whole system is equilibrated at T = 300 K in canonical ensemble (NVT), by applying Nosè-Hoover thermostat [30]. A second equilibration step is performed in