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Thermal behavior of water base-fluid in the presence of graphene nanosheets and carbon nanotubes: A molecular dynamics simulation

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ABSTRACT

This study was examined the thermal behavior of graphene nanosheets/carbon nanotubes-water nanofluid using the molecular dynamics method. First, the atomic stability in simulated structures was investigated by examining kinetic and potential energies. The results of this part represent the convergence of physical quantities. Also, the simulated samples' atomic and thermal behavior was studied by examining independent variables, including the volume fraction and the dimensions of carbon nanoparticles (graphene nanosheets/carbon nanotubes). The molecular dynamics simulations show that with the addition of carbon nanoparticles (NPs) with optimal value (5%), the phase change time and the thermal conductivity of the simulated nanofluid were converged to 1.10 ns and 0.73 W/mK, respectively. Also, increasing the dimensions of carbon NPs leads to a reduction in the phase change time of the simulated structure. Numerically, by increasing the length of carbon NPs to 1 nm, the phase change time in this sample reduces to 1.02 ns? Generally, these results indicate that the thermal behavior of the water-based fluid improved with the addition of carbon NPs.

Nomenclature

F_{ij}	intermolecular force on molecule i by molecule j
m	molecule mass
r	cutoff distance
r_{ij}	position between molecules i and j

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t	time step
r_i	the position of molecule i
v_i	the velocity of molecule i
a_i	the acceleration of molecule i
$J_x(t)$	the heat flux flows
S_i	the system entropy
e_i	the energy
V	the total sample volume
ε	energy parameter in Lennard-Jones (LJ) potential
σ	length parameter of LJ potential
f_A	the repulsive interaction of particles
f_R	the absorption interaction of particles
MD	the molecular dynamics
NVE	the microcanonical ensemble
NVT	the canonical ensemble
NPs	nanoparticle
E_{total}	the total energy

1. Introduction

Nanotechnology is an interdisciplinary science related to materials engineering, medicine, pharmacy, veterinary medicine, biology, semiconductor devices, mechanical engineering, electrical engineering, and chemical engineering [1–10]. Materials have three dimensions a length, width, and height. If at least one of these dimensions is at the nanotechnology scale (1–100 nm), it is called a nanostructure material [11–14]. The thermal properties of the fluid change with the addition of various nanoparticles (NPs) to the base fluid. Physically, adding NPs to the base fluid reduces the specific heat and increases other thermal properties [15]. The study of heat transfer in nanofluids is of great importance and can provide appropriate solutions for optimal heat transfer processes using these structures. Experimental results show that adding various NPs to the fluid significantly increases the heat thermal conductivity of nanofluids. Graphene was first produced experimentally by Novoselov and Geim at the University of Manchester, while graphene-type structures were theoretically investigated in the 1960s [16–19]. Structurally, graphite is graphene plates stacked on top of each other by a van der Waals bond. On the other hand, the carbon particles in a graphene plate are covalently bonded together. During the last decade, much research was performed on simulating fluids and nanofluids' behaviors. Peng et al. and Baratpour et al. [20,21] investigated the effects of temperature and added NPs with different percentages, and expressed the motion characteristics of this nanofluid. The study of particle size in creating the welding process in micro-dimensions is also one of the most important factors that this issue was investigated by Chen [22]. In this work, particles of five different sizes with the diamond structure were studied. The results show that the particle size and the porosity of the walls are also important in the welding process. Using computer simulation, Frank et al. [23] examined the behavior of trapped Ar–Cu nanofluids inside a nanotube. They observed that the thermal conductivity of the nanofluid increases as the NPs volume fraction increases. In another experimental study, Shahsavar et al. [24] examined the thermal conductivity of carbon nanotubes/water nanofluid. In this work, they changed the volume fraction of NPs and the temperature of the structures. The results show that by increasing the temperature and the volume fraction of carbon nanotubes, the thermal behavior of the fluid improves. Yan et al. [25] examined the phase change duration of Ar flow in a microchannel. The results showed the wall's temperature has a direct effect on the phase change process. Zarringhalam et al. [26] studied the thermal behavior of Cu/Ar nanofluid using the molecular dynamics (MD) method. They showed that the addition of NPs has a direct effect on the flow of argon fluid.

This study investigated the thermal behavior of water-based fluid by combining graphene nanosheets and carbon nanotubes by the MD method. By using graphene and carbon nanotubes simultaneously, some disrupted phenomena such as the nanoparticles aggregation process can be managed (modified). This behavior arises from atomic interaction modification between these nanoparticles. In other words, by two type nanoparticles inserting to MD box, attraction force between them has lower ratio rather to carbon nanotube-carbon nanotube and graphene nanosheet-graphene nanosheet interactions. In general, carbon nanotubes have good thermal and chemical stability and a large surface area. But they usually show poor mechanical properties and conductivity [27,28]. On the other hand, due to the high van der Waals forces in carbon nanosheets, these sheets tend to form irreversible aggregations [29,30]. As a result, using carbon nanotube structures and carbon nanosheets overcomes the poor mechanical properties of carbon nanotubes and prevents the aggregations of carbon nanosheets [31,32]. This study was performed using LAMMPS software. Today, LAMMPS software is one of the most common software for performing MD simulations [33–35]. In this research, hypotheses are considered, some of which can be mentioned. The particles present in the simulation box are assumed to be rigid. The simulation temperature and pressure are assumed to be constant and uniform. The number of present particles in the fluid and NPs is assumed to be constant. The simulated carbon NPs are assumed to be rigid. In general, in this study, the effects of the volume fraction and the dimensions of carbon NPs on the thermal behavior of the simulated structures were examined.

2. Computational method

The MD simulation was introduced by Alder and Weinwright [36] and then by Rahman [37]. In this MD simulation, the time course of particle interactions is investigated using Newton's second law as follows [38]:

$$F_i = \sum_{i \neq j} F_{ij} = m_i \frac{d^2 r_i}{dt^2} = m_i \frac{dv_i}{dt} \tag{1}$$

The velocity-Verlet algorithm is the most usual method for integrating motion equations in the MD simulations. In the velocity-Verlet algorithm, the particles' final position and velocity are obtained by integrating the Newtonian equation of motion [39]. Another important factor to consider in the MD simulations is the definition of interatomic forces and potential functions. In MD modeling, the force field is a set of functions and parameters by which the potential energy of a system is estimated [40,41]. To calculate the total potential energy, the applied non-bonded and bonded interactions to the particles must be summed [42]:

$$E_{total} = E_{bonded} + E_{nonbonded} \tag{2}$$

To simulate water molecules in this research, the SPC/E model is used. In this model, interactions are expressed using a simple coordinate oscillator, and nonbonded interactions are expressed using the Lennard-Jones formulation. The Lennard-Jones potential is determined by Eq. (5) [43]:

$$U_{LJ} = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \tag{3}$$

In this formulation, ε and σ are energy and length parameters, respectively. Also, r in this formulation represents the potential cut-off radius. Tersoff potential is appropriate for simulating atoms bound together by covalent bonding. The Tersoff potential function is shown as follow [44]:

$$E = \frac{1}{2} \sum_{i} \sum_{j \neq i} U_{ij} \tag{4}$$

$$U_{ij} = f_C(r_{ij}) \left[f_R(r_{ij}) + b_{ij} f_A(r_{ij}) \right] \tag{5}$$

In these equations, f_A is the expression for their repulsive interaction, and f_R is the expression for the absorption interaction of particles. Thermostats are used to keep the temperature in a constant range [45–47]. In this study, the Nose-Hoover thermostat is used. By applying the Nose-Hoover formulation and considering the velocity-Verlet algorithm, the equations of motion change as follows [45]:

$$r_i(t + dt) = r_i(t) + v_i(t)dt + \frac{1}{2} dt^2 \left[\frac{F_i(t)}{m_i} - \xi(t) v_i(t) \right] \tag{6}$$

$$v_i\left(t + \frac{dt}{2}\right) = v_i(t) + \frac{dt}{2} \left[\frac{F_i(t)}{m_i} - \xi(t) v_i(t) \right] \tag{7}$$

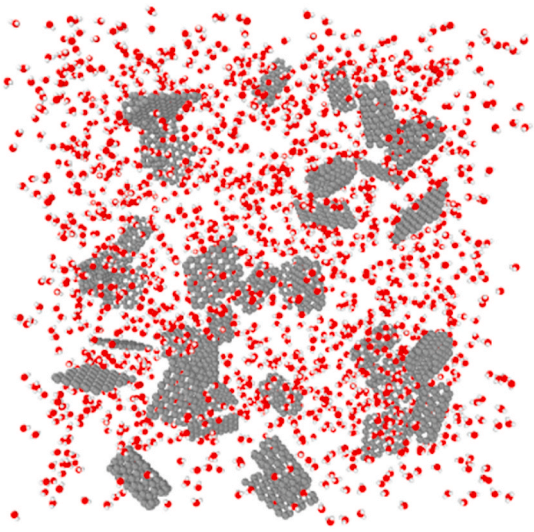

Fig. 1. A view of the simulated nanofluid in the present study.

$$\xi\left(t+\frac{dt}{2}\right)=\xi(t)+\frac{dt}{2Q}\left[\sum_{i}^{N}m_i v_i^2(t)-gk_BT\right] \tag{8}$$

$$\xi(t+dt)=\xi\left(t+\frac{dt}{2}\right)+\frac{dt}{2Q}\left[\sum_{i}^{N}m_i v_i^2\left(t+\frac{dt}{2}\right)-gk_BT\right] \tag{9}$$

$$v_i(t+dt)=\frac{2}{2+\xi(t+dt)dt}\left[dt\frac{F_i(t+dt)}{2m_i}+v_i\left(t+\frac{dt}{2}\right)\right] \tag{10}$$

In the MD simulation, by calculating the heat flux flowing in the atomic samples, the thermal conductivity of the structure can be examined. The heat flux flowing is calculated using the Green-Kubo method [38]. This study investigated the atomic and thermal behavior of water-based fluid in the presence of combined nanosheets of graphene and carbon nanotubes using the MD simulation. For this purpose, a simulation box with dimensions of 10 × 10× 10 nm^3 is considered. The water is considered as the base fluid and is modeled using the SPC/E model. Then, the carbon nanosheets and nanotubes (carbon NPs) are added to the water-based fluid (with the same atomic ratio). Using the Lennard-Jones and Tersoff force field, the simulated structure reaches equilibrium after 1 ns? To control the temperature, the Nose-Hoover thermostat and the NVT ensemble are used. The dimensions of the box in all three dimensions are considered periodically. After ensuring the equilibrate created in the structures, by changing the simulation ensemble to the NVE, the thermal behavior of the simulated nanofluid is investigated after 1 ns? The thermal behavior of the simulated structure is studied by examining the thermal conductivity and the phase change duration of the nanofluid. An example of the simulated atomic structures is presented in Fig. 1.

3. Results and discussion

At first, the equilibration of the atomic structures was investigated by examining kinetic energy and potential energy. Second, the effect of the volume fraction and the dimensions of carbon NPs on the atomic and thermal behaviors of the simulated samples were investigated.

3.1. Thermodynamic equilibrium of simulated structures

In this step, carbon NPs are added to the water-based fluid. Physical quantities such as kinetic energy and potential energy of the atomic system are examined to study the thermodynamic equilibrium in these atomic structures. Fig. 2 represents the kinetic energy changes of the simulated structure. According to Fig. 2, the number of kinetic energy fluctuations decreases with increasing simulation time. Numerically, this quantity converges to 505 eV. From a physical point of view, the convergence of kinetic energy in the studied structures is due to the created temperature equilibrium due to the convergence and reduction of the amplitude of particle oscillations.

Potential energy is another physical quantity that determines the atomic behavior of structures. Fig. 3 represents the potential energy changes of the simulated structure. According to Fig. 3, the numerical value of this physical quantity converged to −75769 eV over time. This convergence in potential energy indicates absorption force in the atomic structure and, consequently, its stability. Increasing the magnitude of this physical quantity is expected to increase the amount of stability in the structures.

Nowadays, researchers are trying to find a suitable solution to increase the stability of various fluids. One way is to add secondary atomic structures such as metal NPs or metal oxides to the base fluid. Also, the study of temperature profiles in simulated samples is very important and shows how the atomic behavior of these structures. Fig. 4 shows the temperature profile of the simulated nanofluid inside the simulation box. According to this diagram, the temperature behavior of the simulated nanofluid is parabolic, and the temperature value of the nanofluid molecules in the center of the simulation box is higher than other space points inside it. The

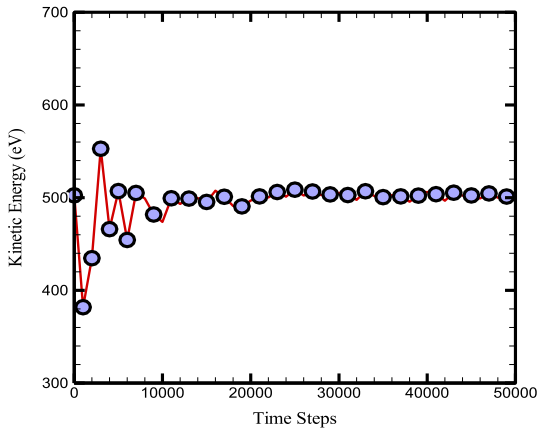

Fig. 2. Kinetic energy changes of the simulated structure, including water molecules and carbon NPs vs. simulation time.

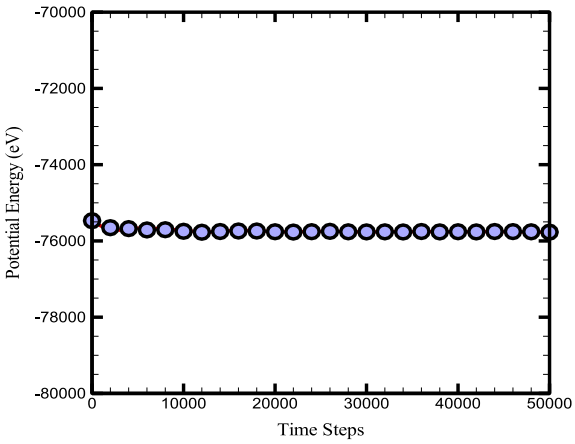

Fig. 3. Potential energy changes of the simulated structure, including water molecules and carbon NPs vs. simulation time.

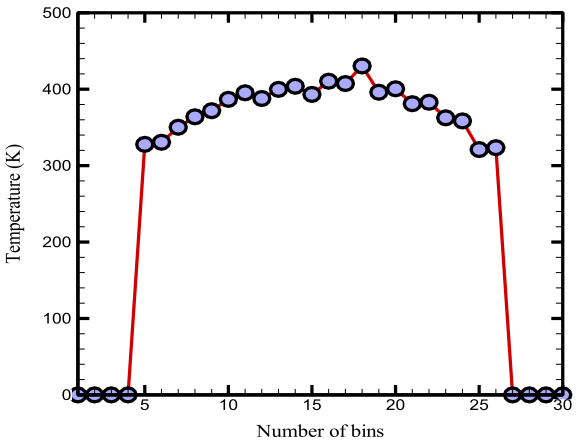

Fig. 4. Temperature profiles in the simulated nanofluid after 50,000-time steps.

dominant physical stability and equilibrium phases arise from simulated structures' base fluid particles (H2O molecules). So, this section doesn't calculate the effects of nanoparticles (graphene and carbon nanotube) of equilibrium phase detection in atomic structures.

3.2. The effect of volume fraction of carbon NPs on the thermal behavior of structures

In this section, the effect of the volume fraction of carbon NPs on the thermal behavior of nanofluid is investigated. The thermal behavior of the nanofluid is investigated by quantities of thermal conductivity and phase change duration. The results of calculating the thermal conductivity of water-based fluid using the Green-Kubo calculation method show that the value of this quantity is equal to 0.63 W/mk, which is very consistent with the results of previous research. On the other hand, the time required to cause a phase change in the simulated atomic sample (base fluid) is calculated at 1.35 ns? Then, with the addition of carbon NPs with atomic ratios of 1, 2, 5, and 10%, the value of the expressed quantities is recalculated. From an operational point of view, the atomic amount of added graphene nanosheets and carbon nanotubes to the water-based fluid is equal to consider the effect of these two factors simultaneously. The obtained values in this part of the research are shown in Table 1 and Figs. 5 and 6. The results show that with the addition of more carbon NPs into the water-based fluid, the thermal behavior of the simulated structure improves. This is physically due to the higher

Table 1
Change in the thermal conductivity and change phase duration of nanofluid at different carbon NPs volume fractions.

Volume fraction (%)	Thermal conductivity (W/mK)	Duration of the phase change (ns)
0	0.63	1.35
1	0.65	1.22
2	0.68	1.18
5	0.73	1.10
10	0.64	1.23

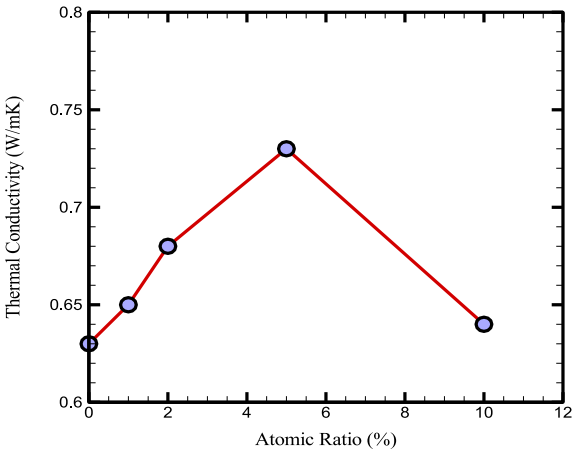

Fig. 5. Changes in thermal conductivity of atomic structure including water molecules and carbon NPs in terms of volume percentage of carbon NPs.

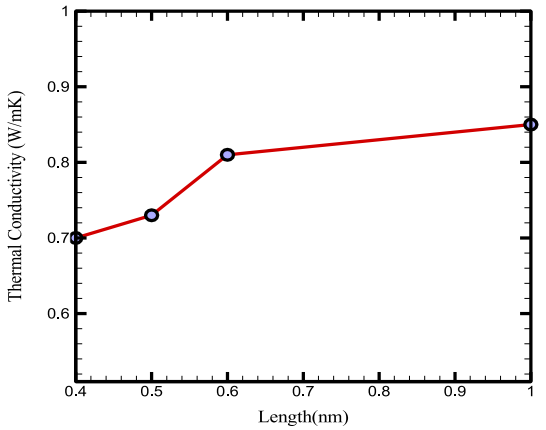

Fig. 6. Changes in the phase change time of the atomic structure, including water molecules and carbon NPs in terms of volume percentage of carbon NPs.

thermal conductivity of carbon NPs than water-based fluid. However, it should be noted that the optimal atomic ratio for adding carbon NPs into the water-based fluid is 5%. On the other hand, As these NPs increase further into the base fluid (up to 10%), the thermal behavior of the simulated nanofluid is disrupted. Therefore, at a higher volume fraction of carbon NPs, clusters are formed and cause sedimentation and reduction of nanofluid stability. As we know, clusters provide a path with less thermal resistance for heat to pass through. Therefore, the optimal state is to add NPs up to a volume fraction of 5%. Numerically, by increasing the volume fraction of carbon NPs up to 5%, the thermal conductivity of the simulated structure increases from 0.63 to 0.73 W/mk; it has increased by about 16%. And the phase change time decreases from 1.35 to 1.10 ns (decreased about 23%).

3.3. The effect of carbon NPs dimensions on the thermal behavior of structures

Considering that the optimal value for improving the thermal behavior of the nanofluid with a volume fraction of 5% carbon nanoparticles, in the continuation, this atomic percentage is used to investigate the thermal behavior of nanofluid. In this step, the effect of carbon NPs length on the thermal behavior of nanofluid is investigated. For this purpose, the thermal behavior of nanofluids in 4 lengths of 0.4, 0.5, 0.6, and 1 was examined. Figs. 7 and 8 represent the changes in thermal conductivity and phase change duration of atomic structure. The results show that increasing the length of carbon nanostructures increases the thermal conductivity, and the duration of phase change in atomic structures decreases. Numerically, increasing the length of simulated carbon NPs to 0.6 nm reduces the conductivity of nanofluid to 0.85 W/mk (increases by about 21%). And the phase change time decreases to a numerical value of 1.02 ns (decreased about 16%). From a physical point of view, as the size of the NPs increases, the surface-to-volume ratio increases, so the atomic interaction between water molecules and carbon NPs increases. Therefore, the thermal behavior of nanofluids is improved by increasing the dimensions of NPs. On the other hand, due to the better thermal behavior of carbon NPs, the improvement of thermal behavior in the initial samples can be seen with the larger NPs. The obtained results are reported in Table 2.

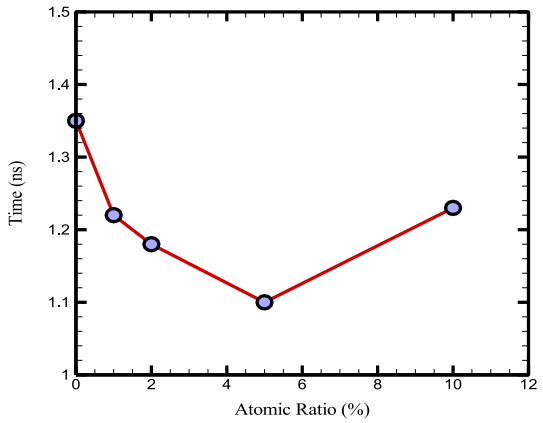

Fig. 7. Changes in thermal conductivity of atomic structure including water molecules and carbon NPs in terms of the length of carbon NPs.

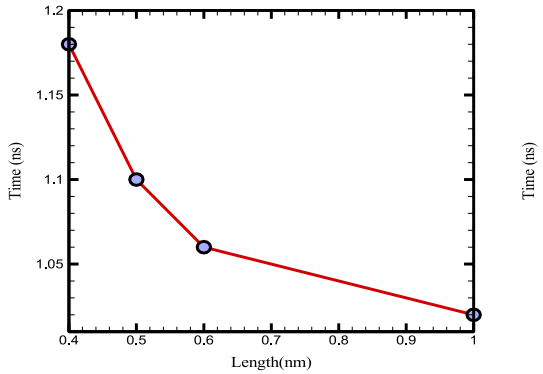

Fig. 8. Changes in the phase change time of the atomic structure, including water molecules and carbon NPs in terms of the length of carbon NPs.

Table 2
Change in the thermal conductivity and change phase duration of nanofluid at different carbon NPs lengths.

Length of carbon NPs (nm)	Thermal conductivity (W/mK)	Duration of the phase change (ns)
0.4	0.7	1.18
0.5	0.73	1.10
0.6	0.81	1.06
1	0.85	1.02

4. Conclusion

This study investigated the atomic and thermal behavior of water-based fluid in the presence of combined carbon NPs using LAMMPS software. At first, the equilibration of the atomic structures was investigated by examining kinetic energy and potential energy. Second, the effect of the volume fraction and the dimensions of carbon NPs on the atomic and thermal behaviors of the simulated samples were investigated. The results of this study are listed as follow:

- In studying the kinetic energy of the simulated structures in the simulation box, the numerical amount of kinetic energy fluctuations decreases with increasing simulation time and converges to 505 eV.
- The numerical value of the potential energy tends to be −75759 eV over time. This convergence in potential energy indicated the presence of absorption in the atomic structure and thus its stability.
- By increasing the volume fraction of carbon NPs up to 5%, the thermal conductivity of the simulated structure increases from 0.63 to 0.73 W/mK. So it has increased by about 16%
- The phase change time in the simulated samples decreases with increasing the volume fraction of NPs. Numerically, adding 5%, carbon NPs decreases the phase change duration from 1.35 to 1.10 ns (was decreased about 23%).

- Increasing the size of NPs is directly related to the thermal behavior of the simulated structures. Increasing the length of the NPs from 0.4 to 1 nm leads to an increase in the thermal conductivity of nanofluid by about 21%. Numerically, the thermal conductivity in the simulated nanofluid increases from 0.7 to 0.85 W/mK.
- Increasing the dimensions of carbon NPs reduces the phase change time in the nanofluid from 1.18 to 1.02 ns (was decreased about 16%).

Finally, we can say the dimension increasing of nanoparticles in this research and applying actual parameters such as atomic defects to nanostructures will be the important challenges in the present study. Experimental research is expected to address these challenges and provide a more comprehensive view of water-based fluid behavior in the presence of carbon nanoparticles.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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