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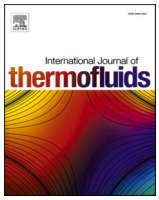

Estimation of thermophysical properties for accurate numerical simulation of nanofluid heat transfer applied to a loop heat pipe

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ABSTRACT

Nanofluids have consistently gained attention over the last decades due to their capability in improving the heat transfer efficiency of thermal devices. This improvement is related to the increase in the working fluid's thermal conductivity when adding solid nanoparticles, also presenting an undesirable influence on other transport properties, such as the increase of the fluid's density, viscosity, etc. To better assess the influence of a certain solid nanoparticle in a base fluid, the obtained data has been used to generate models applied to predict the nanofluids' properties. However, reliability in those models is still a concern as they can show different results for the same characteristics of solid nanoparticles and base fluid, which can generate unreliable data upon applying them in more complex and broad thermal models. A review related to the thermophysical properties of nanofluids is important to offer the basis of analysis for accurate numerical simulation of thermal systems where nanofluids are applied.

Introduction

Nanofluid application is a relatively recent area of investigation with promising results to enhance thermal control devices' performances. Nanofluids are regular working fluids (called base fluid) that have been applied in thermal system devices with solid nanoparticles used to improve the fluids' thermal conductivity. By adding 5% of the working fluid mass with nanoparticles, the liquid thermal conductivity can be increased by up to 20% [1,2]. The first investigations point out that, to have a stable nanofluid without presenting sedimentation, a solid-like nanolayer needs to be formed, which acts as a connection between the solid nanoparticles and the base fluid [3]. The investigations performed in the early stages of nanofluids' development have pointed to the potential of using them in several thermal control applications with great improvement in the heat transfer coefficient. Such improvement was obtained using nanofluids circulating in a loop driven by a regular pump (single-phase), which presents different thermal behavior when compared to systems where the nanofluid needs to go through an evaporation/condensation cycle [4]. In a recent review, Awais et al. [5] tried to provide insight for researchers and designers to incorporate the use of adequate nanofluids while properly understanding the physical phenomenon and the nature of their transport properties. However, as the research in nanofluids advances, several models to predict their thermophysical properties have been proposed, which would be useful to assist in numerical simulations for thermal systems where they are applied. However, due to issues related to different obtained results for the same base fluid, solid nanoparticle, their concentration, etc., it can generate misleading results upon applying them in thermal simulations. Many approaches either theoretical, semi-empirical [6,7] or numerical [8] have been proposed to model the thermo-physical properties of the nanofluids to be then used in the numerical models [9–19]. The objective of this work is to present both the potential of using nanofluids in thermal devices and the concerns involved in using proposed models that can generate diverging results. This is particularly important when it comes to developing and validating numerical models to accurately and realistically simulate the performance of the devices, which use nanofluids as working fluid, to identify optimized solutions [20]. The importance of this topic has also been stated and confirmed by a recent work by Kamenik et al. [21], who numerically investigated the performance uncertainty of heat exchangers operated with nanofluids. This paper presents the models proposed by several authors to estimate the thermal conductivity and the dynamic viscosity of nanofluids, trying to highlight the related uncertainties. Then, a comparison is proposed to show that with a reliable model it is possible to fairly predict the experimental data collected for a loop heat pipe [22]. Heat pipes and

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Nomenclature list

ϕ_p	mass fraction of solid nanoparticles
ϕ_V	volume fraction of solid nanoparticles
ρ_{eff}	nanofluid effective density (kg/m^3)
ρ_l	liquid density (kg/m^3)
ρ_p	particle density (kg/m^3)
μ_{eff}	nanofluid effective viscosity (Pa.s)
μ_f	liquid dynamic viscosity (Pa.s)
k_{eff}	nanofluid effective thermal conductivity (W/m K)
k_f	liquid thermal conductivity (W/m K)
k_p	particle thermal conductivity (W/m K)
D	nanoparticle diameter (m)
Q	heat load (W)
T	absolute temperature (K)
Re	Reynolds number
Pr	Prandtl number

Along with the thermal conductivity, the liquid density requires proper consideration and evaluation in a nanofluid, which can be evaluated according to the two-phase theory [33]:

$$\frac{1}{\rho_{eff}} = \left(\frac{\phi_p}{\rho_p} + \frac{1-\phi_p}{\rho_l}\right), \tag{2}$$

and the liquid dynamic viscosity can be calculated as [32]:

$$\mu_{eff} = \mu_l \frac{1}{(1-\phi_p)^{2.5}}. \tag{3}$$

Eqs. (2) and (3) are important properties used to calculate the overall pressure drop that a system will present, which directly results in the selection of the pump (mechanical system) or capillary evaporator (passive system). When considering a mechanical system, the pump's sizing will directly impact electrical power consumption. In the case of a capillary evaporator used in passive systems, failure to properly evaluate the effects of the transport properties can cause severe loss in performance.

In any case, the most interesting thermophysical properties of nanofluids are the transport ones: thermal conductivity and dynamic viscosity because they are immediately related to the heat transfer enhancement and pressure drop penalization.

For this reason, since the very beginning of the nanofluids' research, thousands of papers have been published, which report experimental data and uncountable models.

Table 1
Thermal conductivity models applied to nanofluids.

Authors	Model	Comments
Koo and Kleinstreuer [34]	$k_{eff} = k_{static} + k_{Brownian}$ $k_{static} = \frac{k_p + 2k_f + 2\varnothing_p(k_p - k_f)}{k_p + 2k_f - \varnothing_p(k_p - k_f)}$ $k_{Brownian} = 5x10^4 \beta \varnothing_p \rho_p c_p \sqrt{\frac{k_B T}{\rho_p D}}(T, \varnothing_p)$	Considers the effects of surrounding liquid motion with random nanoparticles movement. Based on static Maxwell theory and the dynamic effect of Brownian motion
Yu and Choi [3]	$k_{eff} = \frac{k_p + 2k_f + 2\varnothing_p(k_p - k_f)(1+\beta)^3}{k_{pe} + 2k_f - \varnothing_p(k_p - k_f)(1+\beta)^3} k_f$ $k_{pe} = \frac{2(1-\gamma) + (1+\beta)^3(1+2\gamma)\gamma}{-(1-\gamma) + (1+\beta)^3(1+2\gamma)} k_p$	It was based on the Maxwell model but additionally took into account the effects of nanolayer thickness and thermal conductivity parameters
Maxwell [6]	$k_{eff} = \frac{k_p + 2k_l + 2(k_p - k_l)\varphi_p}{k_p + 2k_l - (k_p - k_l)\varphi_p} k_l$	Based on spherical particles, random suspensions must be under conduction solution theory through stationary conditions
Hamilton [7]	$k_{eff} = \frac{k_p + (n+1)k_f + (n-1)\varnothing_p(k_p - k_f)}{k_p + (n-1)k_f - \varnothing_p(k_p - k_f)}$	For high concentrations of spherical particles under conditions of differential effective medium (DEM) theory
Prasher et al. [35]	$k_{eff} = (1 + ARe^m Pr^{0.333} \varnothing_p)\left[\frac{k_p + 2k_f + 2\varnothing_p(k_p - k_f)}{k_p + 2k_f - \varnothing_p(k_p - k_f)}\right] k_f$	Obtained from Maxwell model and included the effects of correction generated by the Brownian motion

loop heat pipes are gaining a lot of interest in many different applications: power generation [23,24], waste heat recovery [25–27] to thermal management of electronic devices [28–32,].

Nanofluids' thermophysical properties evaluation

The thermophysical properties of a nanofluid require a proper adjustment to represent the gain and/or loss of any characteristics due to the addition of nanoparticles. This adjustment requires taking into account the amount of the solid nanoparticles added, considered as a percentage by mass of the base fluid itself. The thermophysical property that is widely discussed among researchers is thermal conductivity, as the addition of solid nanoparticles can represent a substantial gain in this property. Usually, the Maxwell model is applied [6], being this one of the most straight-forward uses for a nanofluid with reasonable accuracy, where Eq. (1) presents the effective thermal conductivity of a homogeneous solution:

$$k_{eff} = \frac{k_p + 2k_l + 2(k_p - k_l)\phi_p}{k_p + 2k_l - (k_p - k_l)\phi_p} k_l. \tag{1}$$

Thermal conductivity of nanofluids

Table 1 presents a review of the contributions from several authors regarding thermal conductivity models applied to nanofluids. From this brief list of thermal conductivity models, it is possible to observe that the correlations vary. When applying the correlations to a given set of nanofluids, with the same base fluid and solid nanoparticles, the results will potentially be different, which will directly impact the final results. When applying any of these models without proper verification, results obtained from simulation models can vary significantly, which may cause misleading interpretations regarding the nanofluid's final thermal behavior.

Important contributions have addressed the interfacial thermal resistances present in nanofluids that also play an important role in

Table 2
Thermal enhancement ratio for CuO and water nanofluids.

Authors	CuO Nanoparticle Size (nm)	Thermal Enhancement Ratio	Volume Fraction (vol%)	Temperature (°C)	Sonication Time (h)
Karthikeyan et al.	8.0	1.020	0.020	20	0.5
[38]	8.0	1.080	0.090	20	0.5
	8.0	1.130	0.100	20	0.5
	8.0	1.190	0.300	20	0.5
	8.0	1.250	0.800	20	0.5
	8.0	1.316	1.000	20	0.5
Nemade et al.	33.0	1.197	0.500	55	1
[39]	42.0	1.134	0.500	55	0.75
	46.0	1.124	0.500	55	0.5
	53.5	1.087	0.500	55	0.25
Khedkar et al.	25.0	1.050	0.010	26	1.5
[40]	25.0	1.120	0.020	26	1.5
	25.0	1.130	0.030	26	1.5
	25.0	1.160	0.040	26	1.5
	25.0	1.170	0.050	26	1.5
	25.0	1.320	0.075	26	1.5
Wang et al.	42.5	1.080	0.020	25	not informed
[41]	42.5	1.100	0.040	25	
	42.5	1.110	0.100	25	
	42.5	1.125	0.150	25	
	42.5	1.160	0.400	25	
Pryia et al.	50.0	1.020	0.004	28	6
[42]	50.0	1.060	0.008	28	6
	50.0	1.100	0.012	28	6
	50.0	1.130	0.016	28	6
	50.0	1.050	0.004	50	6
	50.0	1.160	0.008	50	6
	50.0	1.250	0.012	50	6
	50.0	1.320	0.016	50	6
	50.0	0.950	0.004	55	6
	50.0	1.240	0.008	55	6
	50.0	1.330	0.012	55	6
	50.0	1.430	0.016	55	6

thermal control devices simulations [36], as well as the shear stress effects of nanofluids that are important for pressure drop prediction [37]. The variability in the modeling is due to the great scattering of the available experimental results as it can be inferred from a few results collected from the open literature and listed in Table 2, based on experimental data. The data reported in Table 2 reports the thermal conductivity of nanofluids composed of CuO solid nanoparticles and water as base fluid. It can be observed that there are important differences, considering the same range of solid nanoparticles size, volume fraction added to the base fluid, temperature, sonication time, which leads to a wide range of results. Such a variation in the experimental results for thermal conductivity is also observed for other transport properties and can be considered the most important factor that limits the predicting capabilities of the proposed models.

Besides, there are even other issues in published results that, for example, do not consider chemical incompatibilities between solid nanoparticles and base fluid. The discrepancies observed in the presented experiments/models can result in wrong predictions related to the thermal behavior of a device when using a nanofluid, especially when simulations are utilized to predict its thermal performance.

Dynamic viscosity of nanofluids

As described before, the dynamic viscosity can be considered one of the most important transport properties of a nanofluid. Similar to what was reported for the thermal conductivity, even in the case of dynamic viscosity several different predicting models have been developed and proposed. Table 3 reports a few of the most commonly used models.

Fig. 1 reports the results of the application of a few of the models listed in Table 3, to show how complex can be the proper selection of the equation to be implemented to estimate the dynamic viscosity.

The viscosity ratio is defined to be the ratio between the dynamic viscosity of the nanofluid and that of the base fluid at the same temperature.

While Einstein [43] and Brikman [44] are theoretical models with similar results, this is the reason why Einstein's data points do not show in Fig. 1. The equations proposed by Buongiorno et al. [45] are best-fitting models regressed on datasets for different nanofluids. The black circles show the prediction for Al_2O_3 nanofluid while the red ones refer to Titanium nanofluid. This example confirms that the selection of the model to be implemented needs to be well weighted based on the nanofluid and the operating conditions.

Case study: loop heat pipe operating with nanofluid

This section discusses the results of a simulation model developed to predict the performance of a loop heat pipe (LHP) which uses NiO-water nanofluid as a working fluid. In particular, Eqs (1)-(3) were used to calculate the NiO-water nanofluid properties to verify their effects on the loop heat pipe's (LHP) thermal behavior, to better assess the influence of the addition of the solid nanoparticles to the base fluid and how this would impact the overall LHP's performance [22].

Fig. 2 presents the schematics of an experimental LHP (loop heat pipe) that works passively by generating capillary pressure in the evaporator, using the heat generated by a source. The capillary forces drive the working fluid towards the condenser by the vapor line, where it loses its latent heat and it returns to the liquid phase. The liquid then flows through the liquid line towards the evaporator to complete the cycle. The compensation chamber, which is a two-phase reservoir, self-regulates the amount of working fluid in the system, according to the

Table 3
Proposed dynamic viscosity models for nanofluids.

Authors	Model	Comments
Einstein [43]	$\mu_{eff} = (1 + 2.5\varnothing_p)\mu_f$	Based on a phenomenological hydrodynamic equation for infinitely diluted suspensions of spheres with no interaction between spheres. Works well for maximum volume concentration of 2%
Brinkman [44]	$\mu_{eff} = \frac{1}{(1-\varnothing_p)^{2.5}}\mu_f$	Extended Einstein's model by considering the effect of the addition of one solute molecule to an existing solution.
Buongiorno [45]	$\mu_{eff} = (1 + 39.11\varnothing_p + 533.9\varnothing_p^2)\mu_f$ Al2O3 $\mu_{eff} = (1 + 5.45\varnothing_p + 108.2\varnothing_p^2)\mu_f$ TiO2	Curve fitting from experimental data of Al_2O_3-water and Titania-water nanofluid
Nguyen et al. [46]	$\mu_{eff} = \mu_f 0.904e^{0.148\varnothing_v}$ 47 nm $\mu_{eff} = (1 + 0.025\varnothing_v + 0.015\varnothing_v^2)\mu_f$ 36 nm	Curve fitting from experimental data of Al_2O_3-water nanofluid
Chen et al. [47]	$\mu_{eff} = \mu_f(1 + 10.6\varnothing_v + (10.6\varnothing_v)^2)$	Adjusted model for experimental versus theoretical data by considering the rheological effects of shear-rate
Kulkarni et al. [48]	$ln(\mu_{eff}) = A\left(\frac{1}{T}\right) - B$ $A = 20587\varnothing_p^2 + 15857\varnothing_p + 1078.3$ $B = -107.12\varnothing_p^2 + 53.54\varnothing_p + 2.8715$	Curve fiting from experimental CuO-water: 5%$<\phi_p<$15%, dp=29 nm; 278 $<$ T(K) $<$ 323; shear rate = 100 l/s
Namburu et al. [49]	$log(\mu_{eff}) = Ae^{-BT}$ $A = -0.29956\varnothing_p^3 + 6.738\varnothing_p^2 - 55.444\varnothing_p + 236.11$ $B = -6.4745\varnothing_p^3 + 140.03\varnothing_p^2 - 1478.5\varnothing_p + 20341$	Curve fitting from experimental data of Al2O3-ethylene-glycol nanofluid: 1% $<\phi_p<$10%; dp=53 nm; 278K$<T<$323 K
Abedian et al. [50]	$\mu_{eff} = \frac{\mu_f}{(1-\frac{5}{2}\varnothing_p)}$	Extention of Einstein's equation for obtaining good agreement in volume concentration ranges of up to 18–20% in suspension system non-interacting with spherical particles.

applied power to the evaporator [22]. The geometric characteristics of the LHP used for this verification are presented in Table 4. The LHP was built with 316 L stainless steel.

Mathematical simulations have been performed to check the results with the experimental tests, for the cases with water and water-NiO nanofluid. The development of two-phase thermal control devices using nanofluids, such as the presented LHP, is part of a wider project to promote the effective thermal management of sensitive electronic equipment. Therefore, some detailed information is not presented because it is considered proprietary, which is the case of detailing the mathematical model employed here.

Fig. 3 presents the comparison between the simulation and experimental results for the LHP operating with water and NiO-water nanofluid (addition of 3.5% wt.-% of NiO solid nanoparticles, 99.5% purity) with a mean diameter of 40 nm. The nanofluid was prepared with a 2-step method, where the base fluid and the nanoparticles were mixed in an ultrasonic bath for 10 h to ensure its stability. Surfactants were not applied since this practice must be avoided in systems operating in saturation conditions due to the potential enhancement of chemical reactions that will generate non-condensable gasses (NCGs) that causes a negative impact on the LHP's thermal performance [51,52].

The experimental verification was performed by testing the LHP with each working fluid, where the temperatures throughout the testing setup were measured with type-T thermocouples. The experimental results were then used to validate the simulation model, and to verify the agreement between the results. The LHP model is based on the thermal and hydraulic balances according to the heat loads applied to the evaporator. Temperature and pressure drop throughout the LHP are calculated simultaneously to predict its thermal behavior. The temperature calculations are used in each interaction to determine the working fluid's transport properties, which are then used to determine the pressure drop in each component of the LHP as presented in Fig. 2 [22]. In the case of nanofluids, Eqs. (1) to (3) are used to determine the effective thermal conductivity, density, and viscosity, respectively.

The simulated and experimental results present an acceptable agreement, showing that the LHP's heat source temperature (evaporator) is lower when only using the base fluid. When using the nanofluid, the evaporator temperature increases due to the increase of the overall pressure drop observed throughout the LHP. All calculations were performed using the so-called classical models applied to nanofluids, showing good agreement between the experimental and calculated results.

When performing the same simulations with any other proposed model, the calculations became unstable, and the simulations diverged or presented misleading results, which lead to the conclusion that the proposed models still require refinements to present reliability during calculations. Such behavior is expected when applying the presented models in simulations that are carried out for other thermal control devices, with either active or passive pumping actions. The difference in the results when applying a model that incorrectly predicts the nanofluid's properties can significantly impact its correct analysis.

Conclusions

Nanofluids are potential elements in enhancing the heat transfer capabilities of thermal devices. There are several models available that claim to predict a nanofluid thermophysical property capability, but issues are found in many of them as different results are obtained for the same nanofluid. The variability on the different experimental datasets reported in the open literature explains why so many models have been proposed so far to predict the most important transport properties of nanofluids: thermal conductivity and dynamic viscosity. As shown for both properties, the models show unreliable and quite scattered results even for the same nanoparticle and concentration. In the case of the dynamic viscosity, it was demonstrated that the kind of nanoparticle deeply affects the predicted values. This implies that the selection of the most suitable model to predict the thermophysical properties depends upon the experience of whom is called to perform those analyses.

When verifying the so-called classical models during a simulation of an LHP to predict its thermal performance, the obtained results showed good agreement with the ones observed during the testing program. However, when applying any other proposed model, the simulations presented stability issues during the calculations as well as misleading results. Therefore, the proposed models still require proper treatments to be applied in simulation and/or designing tools for thermal management systems.

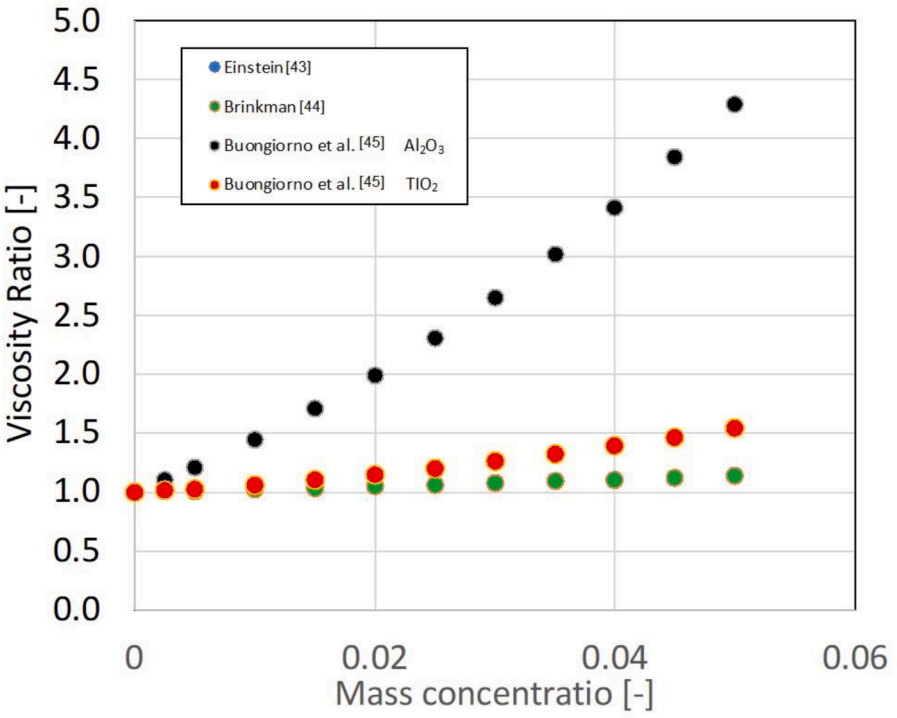

Fig. 1. Viscosity ratio as a function of the mass concentration.

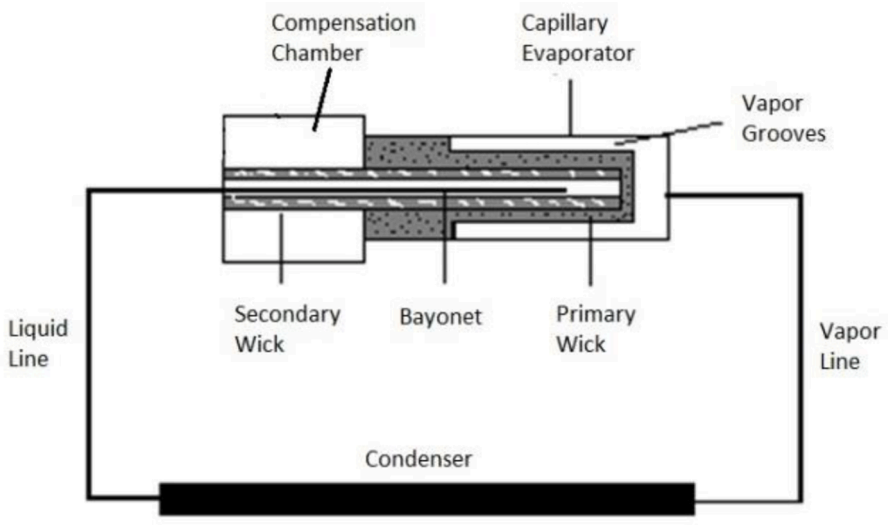

Fig. 2. Schematics of an LHP (Source: GamaTech Thermal Solutions).

Table 4
Geometric characteristics of the LHP (Source: GamaTech Thermal Solutions).

Capillary Evaporator	Liquid Line	Vapor Line
Heat removal area: 3.0 cm^2	OD/ID(mm): 3.0/1.5	OD/ID(mm): 3.0/1.5
Number of grooves: 10	Length: 300 mm	Length: 200 mm
Nickel Wick Structure	Compensation Chamber	Condenser
Mean Pore size: 3 μm	Total Volume: 6 cm^3	OD/ID(mm): 3.0/1.5
Porosity: 75%		Length: 500 mm

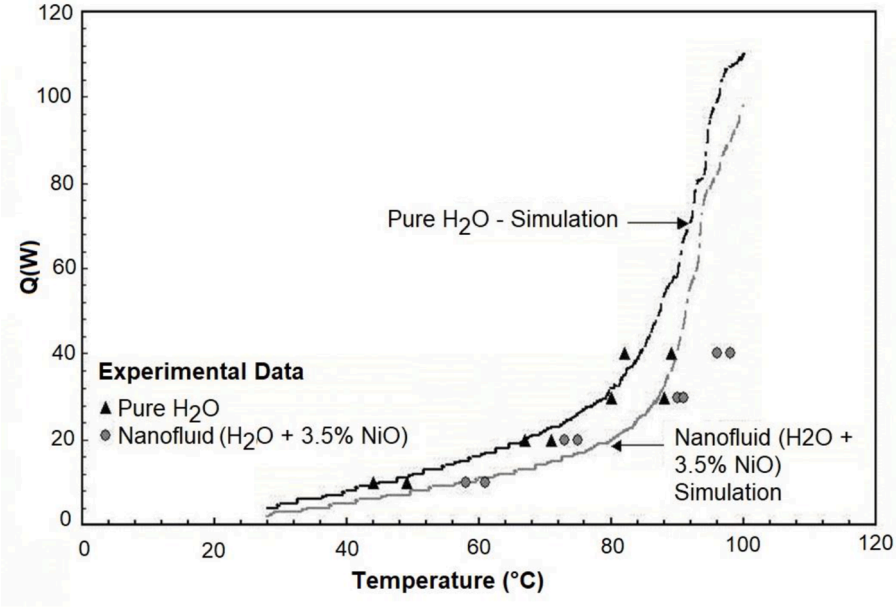

Fig. 3. LHP operation comparison: experimental and simulated results (Source: GamaTech Thermal Solutions).

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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