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CFD ANALYSIS OF PEG 400 BASED NANOFLUIDS

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Abstract: In the last years, a lot of research is dedicated to development of new heat transfer fluids. Phase change materials (PCM) are considered a new generation of heat transfer fluids. A convenient tool to verify the efficiency of a fluid PCM for different practical applications is the simulation approach. In order for such an analysis to be possible, it is necessary to correctly and completely describe the fluids, which supposes the knowledge of the laws of variation of the thermophysical properties with temperature. In many industrial applications, heat transfer is one of the most significant process, but the development of efficient equipment is limited by the low thermal conductivity of conventional heat transfer fluids. Complex CFD (computational fluid dynamics) programs, such as ANSYS Fluent, are capable of replacing experimental results. Therefore, based on previous experimental data, a numerical study on heat transfer will be performed, involving laminar flow conditions. In this numerical study, a number of nanofluids based on PEG 400 (polyethylene glycol PEG 400) and two type of nanoparticles (Al_2O_3 and ZnO), have been implemented in a commercial code to analyze their behavior at heating. Their heating behavior must be understood under different conditions or factors, such as concentration, temperature, pressure, flow conditions, heating systems and flow geometry. In conclusion, PEG 400 based nanofluids is considered to have a high potential for a number of practical applications (for example for their possible use in thermal energy storage), but further studies are needed, as well as the intensification of numerical and experimental research because no applied studies have been identified in the literature.
Key words: CFD, nanofluids, phase change materials, polyethylene glycol.

1. INTRODUCTION

The opportunity for experimental research in the field of nanofluids arose as a result of the high need to improve heat transfer in various industrial applications, by creating and characterizing new heat transfer fluids. Phase-changing materials (PCMs) have low thermal conductivity, which limits their use and with the addition of nanoparticles with high thermal conductivity, these new fluids, known as nano-PCMs, have emerged. Marcos et al. (Marcos et al., 2019. Marcos et al., 2020. Marcos et al., 2018) discussed about the thermal conductivity of several nano-PCMs that had as base fluid PEG 400 (polyethylene glycol PEG 400) and three types of nanoparticles (MWCNT, GnP, Ag). During the studied temperature range, the thermal conductivity decreased slightly with increasing temperature and the thermal conductivity of the nanofluid increased with the concentration of nanoparticles. Chereches et al. (Chereches et al., 2017) measured the thermal conductivity of PEG 400 nano-enhanced with Al_2O_3, ZnO and MWCNT. They observe an improvement in thermal conductivity depending on the concentration of nanoparticles. Regarding numerical studies, it is absolutely necessary to determine in the first phase the thermophysical properties of fluids and their variation with temperature, thus creating the premises for a correct numerical analysis. In the following, studies on the numerical analysis of nanofluids enhanced with nanoparticles in suspension will be presented. To the knowledge of these authors, studies on the numerical analysis of nano-PCM are limited, so the results obtained on nanofluids and ionanofluids will be discussed. Chereches et al. (Chereches et al., 2017) published an article on the laminar and turbulent behavior of a number of 8 fluids enhanced with alumina nanoparticles, based on two ionic liquids. The numerical study was performed on a tube-type geometry, in 3D, using the Ansys Fluent software. Also, Chereches et al. (Chereches et al., 2017, Chereches et al., 2021, Chereches et al., 2020) performed numerical analyzes that took into account a laminar flow regime (due to the high viscosity of ionic liquids) and various practical situations of application of heat flux, for example: along the entire length of the tube (Chereches et al., 2017), in the middle of the tube (Chereches et al., 2021) or only at the outlet of the fluid from the tube (Chereches et al., 2020). Minea (Minea, 2017) observed convective heat transfer coefficient enhancement of 257 % for hybrid nanofluid with 2.5 % Al_2O_3 + 1.5% SiO_2 dispersed in water. Paul et al. (Paul et al., 2015) found the convective heat transfer performance is higher for the NEILs (nanoparticle-enhanced ionic liquids) (with Al_2O_3 nanoparticle enhanced) with almost 27 % compared with base ionic liquid. Azmi et al. [10] determined for TiO_2 and SiO_2 nanofluids a heat transfer enhancement with 26% for 1.0% volume concentration. In this paper, a numerical study was performed through CFD (computational fluid dynamics) - type programs of the behavior in operation of new experimentally developed fluids. The nano-PCM prepared are based on polyethylene glycol PEG 400 in which two types of oxide nanoparticles have been added.

2. NUMERICAL APPROACH

Numerical analysis is a method widely used in recent years in many scientific studies, being extremely useful in the preliminary assessment of the behavior of a fluid in a practical application. The numerical simulation was performed in laminar flow regime in a pipe for different nanofluids with two type of nanoparticles (Al_2O_3 and ZnO). All the details about the problem specification are presented in Table 1 and the pipe cross section and more details about the description of the case can see in Chereches et al. [6] and the CFD software used is Ansys Fluent [11]. The velocity of each fluid was calculated based on the Reynolds number.

$$Re = \frac{w \cdot d}{\nu} \qquad (1)$$

where: w is the average fluid velocity (m/s), d is the characteristic length of the flow (m), υ is the kinematic viscosity of the fluid (m^2/s).

Table 1. Problem specification (Chereches et al 2021).

Pipe radius	$2.94.10^{-2}$ m
Pipe length	6.045 m
Temperature	298.15 K
Outlet Pressure	97225.9 Pa
Wall heat flux	5210.85 W/m^2
Ambient pressure	98338.2 Pa
Heating area	x = 1.83 m and x = 4.27 m

Numerical analysis involves the creation of a system of differential equations that will be solved under the imposed conditions, with reference to the initial conditions, final and contour conditions, but also the properties of the fluid. All of these equations are described in Chereches et al. (Chereches et al., 2021). Incorporation of nanoparticles into the base fluid leads to a change in the thermophysical properties, such as thermal conductivity, viscosity, density and specific heat, which affect convective heat transfer. The nanoparticles concentration, purity level, nanomaterial shape and size are some of the main factors that significantly modify the thermophysical properties of nanofluids. The thermophysical properties of all the heat transfer fluids used in this study were experimentally measured by Chereches et al. ((Chereches et al., 2020, Chereches et al., 2021) and table 3 summarizes the previous experimental results of the fluids used in this study. Only the fluid density was theoretically determined using the Pack and Cho equation (Pac and Cho, 1998):

$$\rho_{nf} = \phi_{vol}\rho_p + (1 - \phi_{vol})\rho_{bf} \qquad (2)$$

where: ρ_{nf} is density of nanofluids (Kg/m^3), φ_{vol} is volume fraction of nanoparticles, ρ_p is density of the nanoparticles (Kg/m^3),, ρ_{bf} is denstity of base fluid (Kg/m^3).

3. RESULTS AND DISCUSSION

The results of the numerical analysis will be discussed in terms of improved heat transfer, variation of pumping power, as well as performance evaluation criteria to outline a complete analysis of the behavior of fluids in tube heating.

Heat transfer efficiency

Heat transfer was analyzed using a convective heat transfer coefficient for all fluids implemented in numerical analysis using Ansys Workbench CFD software. On the other hand, the heat transfer improvement was calculated using the relative convection heat transfer coefficient, which is defined as the ratio between the convective heat transfercoefficient of the nanofluids and the base fluid as follows:

$$h_r = \frac{h_{nf}}{h_{bf}} = \frac{Nu_{nf} \cdot k_{nf}}{Nu_{bf} \cdot k_{bf}} \qquad (3)$$

Table 2. New fluids and their codes (Chereches et al. 2020, Chereches 2020, Chereches et al 2021).

Fluid type	Code	Mass concentration	Mass fraction	Volume fraction
Base fluid	PEG 400	0.00	0.000	0.00000
Nano fluid	0.50 % Al_2O_3	0.50	0.005	0.00142
	1.00 % Al_2O_3	1.00	0.010	0.00285
	2.50 % Al_2O_3	2.50	0.025	0.00721
	0.50 % ZnO	0.50	0.005	0.00101
	1.00 % ZnO	1.00	0.010	0.00202
	2.50 % ZnO	2.50	0.025	0.00512

Table 3. Thermophysical properties of base fluid and nanofluids at 298.15 K (Chereches et al., 2020, Chereches, 2020, Chereches et al., 2021).

Code	Specific heat (J/Kg*K)	Density (Kg/m^3)	Thermal conductivity (W/m*K)	Dynamic viscosity (N-s/m^2)	Kinematic viscosity (Kg*m/s)
PEG 400	2363.00	1125.00	0.190	0.124	1,10e-04
0.50 % Al_2O_3	2471.65	1127.02	0.191	0.129	1,14e-04
1.00 % Al_2O_3	2490.00	1133.12	0.191	0.132	1,16e-04
2.50 % Al_2O_3	2510.00	1145.52	0.194	0.139	1,21e-04
0.50 % ZnO	2359.15	1129.51	0.199	0.130	1,15e-04
1.00 % ZnO	2404.33	1134.06	0.204	0.130	1,15e-04
2.50 % ZnO	2410.16	1147.94	0.209	0.129	1,12e-04

where: *r* refers to relative, *k* refers to thermal conductivity, indices *nf* to the new fluid and *bf* to the base fluid. In this idea, in Figure 1 present the fluid type influence on Nu number (Nu) at different Reynolds number (Re). Variation of the relative heat transfer coefficient with the Reynolds number for 1% wt nanofluids is represented in Figure 2. It can be seen that the addition of ZnO nanoparticles, the heat transfer is enhanced by 15% for both Reynolds number.

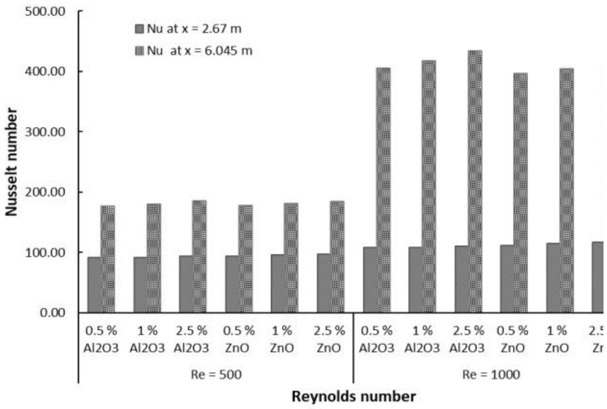

Fig. 1. Nusselt number variation versus Reynolds number, at x = 2.67 m and 6.045 m.

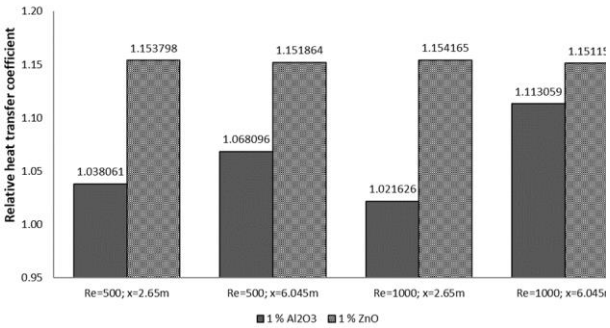

Fig. 2. Heat transfer coefficient enhancement for two nanofluids.

On the other hand, the heat transfer is improved by up to 6% for Al_2O_3-based nanofluids for Re = 500 and by 11% for Re = 1000.

Figure 3 shows information on the wall temperature, which was numerically evaluated for the two areas (at x = 2.67 m and x = 6.045 m). The wall temperature decreases at the outlet and the best results were obtained for nanofluids with a mass concentration of 2.5% wt at Re = 1000. It should be noted that a low temperature means a more efficient convection heat transfer.

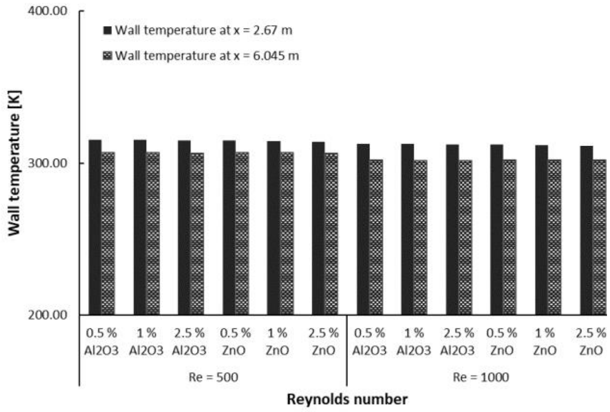

Fig. 3. Wall temperature evaluation.

Pumping power

Pumping power has a relevant effect in estimating total energy consumption for any practical application. Thus, if we consider the basic equations in fluid mechanics, the pumping power can be calculated with the equation [4]:

$$W = \dot{v}\Delta P = w\frac{\pi D^2}{4}\left(f\,\frac{L}{D}\,\frac{\rho w^2}{2}\right) \tag{4}$$

where: $\dot{v}$ is the volume flow, ΔP is the pressure difference in the pipe, w is the fluid velocity, f is the coefficient of friction, ρ is the density and L, D represents the length, respectively the diameter of the pipe.

To facilitate the presentation of the results, the relative pumping power (W_r) is defined as the ratio between the pumping power of the nanofluid (W_{nf}) and the pumping power of the base fluid (W_{bf}), as follows:

$$W = \frac{W_{nf}}{W_{bf}} \tag{5}$$

where: r refers to relative, indices nf refers to the new fluid and bf to the base fluid.

Figures 4 and 5 show that the addition of nanoparticles to the base fluid causes an increase in pumping power as the concentration of nanoparticles increases. On the other hand, the same phenomenon applies to both Reynolds numbers considered in this study. It can also be seen that the pumping power is the same for both areas studied.

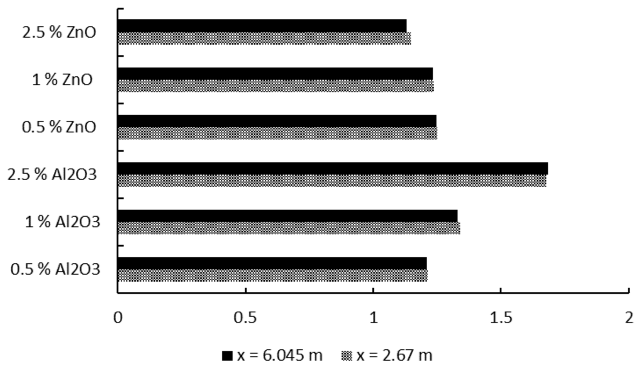

Fig. 4. Relative pumping power for nanofluids for Re = 500

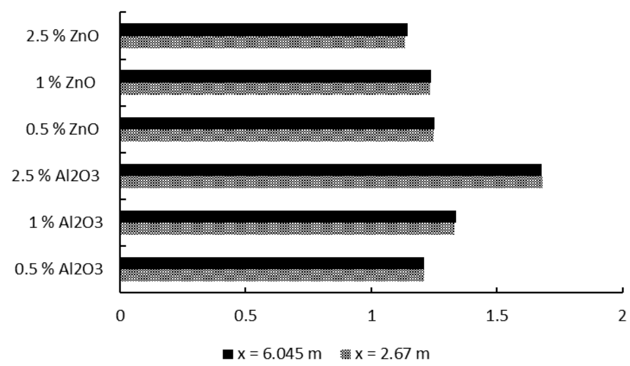

Fig. 5. Relative pumping power for nanofluids for Re = 1000

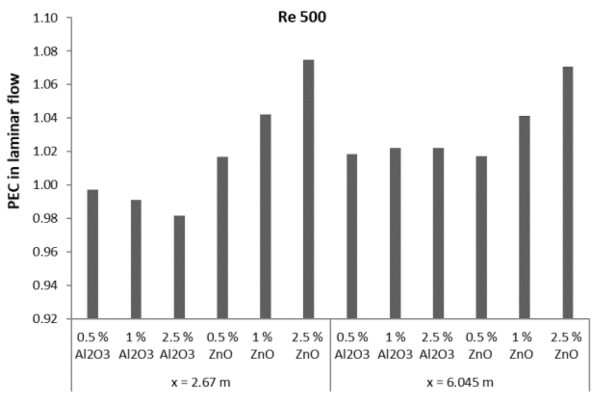

Fig. 6. Results on performance evaluation criterion for studied nanofluids at x = 2.67 m and x = 6.045 m for Re = 500

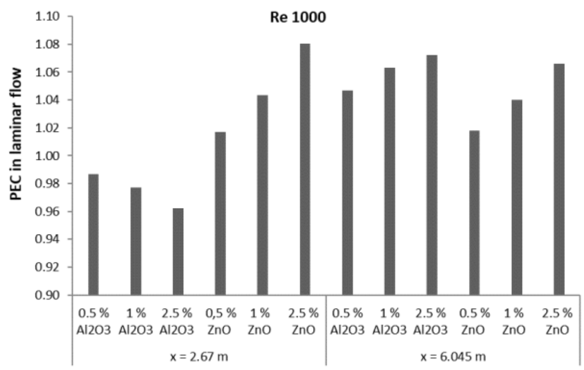

Fig. 7. Results on performance evaluation criterion for studied nanofluids at x = 2.67 m and x = 6.045 m for Re = 1000

Performance evaluation criteria

The performance evaluation criterion (PEC) has also been studied who take into account the improvement Nu with the simultaneous increase of the friction factor and is defined as (Webb and Kim, 2006):

$$PEC = \frac{\left(\frac{Nu_{nf}}{Nu_{bf}}\right)}{\left(\frac{f_{nf}}{f_{bf}}\right)^{1/3}} \qquad (6)$$

where: *Nu* refers to Nusselt Number, *f* refers to friction factor, indices *nf* refers to the new fluid and *bf* to the base fluid.

This criterion takes into account the improvement of the Nusselt number in terms of the friction factor (from simulation) and the flow rate is improved when PEC > 1. The results are presented in Figure 6 and 7. It can be seen that the fluids have very good performances in terms of Nusselt number and friction factor, but the best results were collected at x = 6.045m.

4. CONCLUSIONS

A numerical analysis was performed to estimate the thermal transfer performance of polyethylene-glycol PEG 400 with Al_2O_3 and ZnO nanoparticles added in mass concentration of 0.50 % wt, 1.00 % wt and 2.50 % wt. As a general observation, it can be stated that the numerical results depends a lot on the type and concentration of nanoparticles in the base fluid, as well as Reynolds' number. ZnO-based nanofluids perform better in heat transfer than Al_2O_3-based nanofluids, which is influenced by the higher thermal conductivity of these nanofluids. Also, the heat transfer coefficient increases with the addition of nanoparticles to the base fluid and with Re increasing. The wall temperature was numerically evaluated and in the middle of the pipe (at x = 2.67m) the wall temperature is higher, this means the decrease in exit wall temperature shows an increase in heat transfer inside the pipe. If it talks about the pumping power, it depends on the type of nanoparticle but also on their concentration. However, the results obtained need to be verified in practice, and further studies, both numerical and experimental, are needed to verify these hypotheses and to be able to draw a solid conclusion about the possible use of nano-PCM as a new heat transfer fluid.

5. ACKNOWLEDGMENTS

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6. REFERENCES

1. Marcos, M.A., Podolsky, N.E., Cabaleiro, D., Lugo, L., Zakharov, A.O., Postnov, V.N., Charykov, N.A., Ageev, S.V., Semenov, K.N., (2019). *MWCNT in PEG-400 nanofluids for thermal applications: A chemical, physical and thermal approach,* Journal of Molecular Liquids, 294, 611-616.
2. Marcos, M.A., Cabaleiro, D., Hamze, S., Fedele, L., Bobbo, S., Estellé, P., Lugo, L., (2020). *NePCM Based on Silver Dispersions in Poly(Ethylene Glycol) as a Stable Solution for Thermal* Storage, Nanomaterials, 10(1), 19.
3. Marcos, M.A., Cabaleiro, D., Guimarey, M.J.G., Comuñas, M.J.P., Fedele, L., Fernández, J., Lugo, L., (2018). *PEG 400-Based Phase Change Materials Nano-Enhanced with Functionalized Graphene Nanoplatelets,* Nanomaterials, 8(1), 16.
4. Chereches, M., Vardaru, A., Huminic, G., Chereches, E.I., Minea, A.A., Huminic, A., (2022). *Thermal conductivity of stabilized PEG 400 based nanofluids: An experimental approach,* International Communications in Heat and Mass Transfer, 130, 105798.
5. Chereches, E.I., Sharma, K.V., Minea, A.A., (2017). *A numerical approach in describing ionanofluids behavior in laminar and turbulent flow,* Continuum Mechanics and Thermodynamics, 30, 657-666.
6. Chereches, E.I., Chereches, M., Alexandru, A., Dima, A., Minea, A.A., (2021). *Nanoparticles in ionic liquids: numerical evaluation of heat transfer behaviour in laminar flow,* Heat Transfer Engineering, 42, 1625-1634.
7. Cherecheş, E.I., Minea, A.A., Sharma, K.V., (2020). *A complex evaluation of [C2mim][CH3SO3] – alumina nanoparticle enhanced ionic liquids internal laminar flow,* International Journal of Heat and Mass Transfer, 154, 119674.
8. Minea, A.A., (2017). *Hybrid nanofluids based on Al_2O_3, TiO_2 and SiO_2: Numerical evaluation of different approaches,* International Journal of Heat and Mass Transfer, 104, 852–860.
9. Paul, T.C., Morshed, A.K.M.M, Fox, E.B., Khan, J.A., (2015). *Thermal performance of Al_2O_3 Nanoparticle Enhanced Ionic Liquids (NEILs) for Concentrated Solar Power (CSP) applications,* International Journal of Heat and Mass Transfer, 85, 585-594.
10.Azmi, W.H., Sharma, K.V., Sarma, P.K., Mamat, R., Najafi, G., (2014). *Heat transfer and friction factor of water based TiO2 and SiO2 nanofluids under turbulent flow in a tube,* International Communications in Heat and Mass Transfer, 59, 30-38.
11.*ANSYS Fluent Tutorial Guide 2020 R2*, pdf, http://www.pmt.usp.br/academic/martoran/notasmodelosgrad/ANSYS%20Fluent%20Users%20Guide.pdf, accessed: 21.10.2021.
12. Chereches, M., Bejan, D., Ibanescu, C., Danu, M., Chereches, E.I., Minea, A.A., (2021). *Viscosity and isobaric heat capacity of PEG 400-Based Phase Change Materials Nano-Enhanced with ZnO nanoparticles,* Journal of Thermal Analysis and Calorimetry, 147, 8815–8826.
13. Chereches, M., Ibanescu, C., Danu, M., Chereches, E.I., Minea, A.A., (2021). *PEG 400-Based Phase Change Materials Nano-Enhanced with Alumina: an experimental approach,* Alexandria Engineering Journal, 61(9), 6819-6830.
14. Pak, B.C., Cho, Y.I., (1998). *Hydrodynamic and heat transfer study of dispersed fluids with submicron metallic oxide particles,* Experimental Heat Transfer, 11, 151–170.
15. Minea, A.A., (2020). *Pumping power and heat transfer efficiency evaluation on Al_2O_3, TiO_2 and SiO_2 single and hybrid water-based nanofluids for energy application,* Journal of Thermal Analysis and Calorimetry, 139, 1171–1181.
16. Webb, R.L., Kim, N.H., (2004). *Principles of Enhanced Heat Transfer,* 2nd ed., Garland Science, New York.

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