Prediction of thermal distribution and fluid flow in the domain with multi-solid structures using Cubic-Interpolated Pseudo-Particle model

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Abstract

A nanofluid is a suspension of very small solid particles in a continuous fluid with significant improvement of heat transfer characteristics in the main liquid. In general, in industrial equipment, the heat transfer rate can be improved with optimization of equipment including the domain structure and using the different types of nanofluids. Still, there is a big challenge to analyze the heat transfer and fluid circulation in the domain. Having nanofluids with experimental observation as using sensors and probes are destructive for the liquid stream and they are costly to observe the details of particles and the original fluid. Over the 20 years, different numerical methods have been implemented in the modeling of the heat and fluid distribution in industrial equipment containing nanofluids. Among all mathematical and numerical methods, Cubic-Interpolated Pseudo-Particle (CIP) model provides a strong potential in the prediction of the fluid structure and heat analysis, when there is a complex structure of thermal walls and high concentration of nanoparticles. However, this method is not frequently used by researchers in nanofluids analysis. In this study, the Cubic-Interpolated Pseudo-Particle model is applied to predict the flow in the square domain. different thermal walls (multi-solid structure) and hot cylindrical wall are specifically used to observe the fluid flow and heat distribution in the domain. Additionally, for a better understanding of the flow in the domain, different numbers of cylinders are used and also different amounts of nanofluid in the continuous fluid are added. The results show that adding more walls in the domain causes the change in the vortex structure. Furthermore, using nanofluid results in better heat transfer rate in the system. The CIP method is also a capable tool to predict the heat and fluid flow in the multi-solid structure domain.
1. Introduction

It is well perceived that although numerous industrial techniques are applied to increase heat transfer, the low amount of process fluid’s thermal conductivity prevents great compactness and effectiveness of heat transfer equipments. A novel and promising procedure to improve the thermal conductivity of fluids is to apply small solid particles in the fluids [1].

To make heat transfer equipment less energy consuming, it is necessary to reach a massive increase in heat flux and diminish its dimensions. Heat transfer in fluids has a critical role in various applications such as chemical processes, power generation, reactor insolation, heating or cooling processes, microelectronics, membrane contactors, solar collectors, cooling of the electronic devices and home ventilation [2–10].

Such equipment must be designed in a way that it can provide the highest thermal efficiency and lowest size. In this regard, the small thermal conductivity of conventional coolant materials including water oil and ethylene glycol is a serious obstacle. For example, to achieve a certain thermal efficiency in a double tube heat exchanger, it is necessary to increase the heat exchanger length when a decrease occurs in the coolant’s thermal conductivity [11, 12]. Here, using nanofluids to enhance the heat transfer rate provides some advantages like size reduction in the fabricated heat transfer system, improvement in heat transfer, reduction in cost and weight of the fabricated thermal equipment, the least clogging, apparatus miniaturization, and microchannel cooling [13–16].

The low-quality heat analysis features of main liquids in comparison with most solids introduce a major problem to the efficiency of industrial equipment. Hence, numerous efforts have been made for the preparation of ultrafine solid materials with a thermal rate more significant than the commonly used liquids [17–19].

Suspending nanoparticles can be considered as a novel idea in improving the industrial equipment. Several materials such as polymeric, metallic, and non-metallic particles are added to fluids for making some slurries. Nevertheless, the typical slurries with particles in the size range of micrometers (μm) to millimeters (mm) would probably lead to some serious issues [20, 21]. The abrasion caused by these particles leads to erosion of pipelines and clogging of flow channels. Moreover, their suspensions frequently have to deal with rheological and instability issues because of the inclination of the particles to rapid settlement. Hence, despite the higher thermal conductivities of the slurries, they are not practical [22, 23].

A set of experimental works have indicated a considerable growth in heat transfer in a nanofluid containing aluminum or copper nanoparticles suspended in mineral oils or even water. Despite an increasing body of works conducted on heat transfer increase and nanofluids, many of them still have difficulties dealing with the macroscopic phenomenon occurring inside the nanofluid. Thus, they provide little information about the micro-scale enhancement mechanism of energy transport [24–26].

Generally, liquid molecular particles surround the solid nanoparticles suspended in a base liquid. These solid nanoparticles are always bombarded with the surrounding liquid particles. In addition, solid particles interact constantly. During the nanofluid preparation, some surface dispersants are applied to obtain stable nanoparticles with even distributions. These dispersants, in turn, lead to a set of complicated interactions between the liquid and solid particles. By exerting some internal and external forces, the suspended nanoparticles move irregularly even if the suspension is stationary at a microscopic scale [27, 28]. For instance, Brownian force put the nanoparticles in Brownian motion while gravitational forces lead to their sedimentation. The random motion of the nanoparticles may be accompanied by the aggregation of the particles. Here, the aggregation of the solid ones may occur because of the interaction of the nanoparticles. All nano characteristics play a key role in controlling the energy transport.
and flow processes in a given nanofluid [29–31]. Eastman et al conducted some experimental investigations about the influence of solid nanoparticles addition to fluid on the thermal conductivity. They corroborated that the addition of 5 vol.% CuO nanoparticles to water resulted in increasing its thermal conductivity by approximately 60% [32].

Many numerical methods have been used in the prediction of the nanofluids in industrial structures [33–36]. In the present study, the CIP method is employed as an efficient method for handling the heat transfer analysis in square shape domain with multi-solid structure with hot walls. Additionally, this method is used to model the nanofluid in the multi-structure domain.

2. Method

The square shape domain is used to simulate the liquid flow and heat distribution in this study. The right and left walls represent a hot and cold wall, while the top and bottom walls illustrate adiabatic walls. In this study different multi-solid walls are used for examining the CIP method in prediction of thermal distribution in the domain. The first structure is one cylindrical solid domain in the domain, and for the multi-structure domain, the triple cylinders are considered in simulations. At the beginning, the air is simulated in the domain, but after that water is mixed with Silicon Dioxide (TiO₂) and add it into the domain with one object for observation of the thermal distribution and liquid stream.

To calculate the heat distribution and fluid flow, the CIP method is used in this study. Due to the flexibility of this method for nonlinear computing problems, this method splits the hyperbolic equation into two different stages including advection and non-advection. the voracity and energy equations in the two-dimensional cavity are calculated. The cavity domain has been also used in several studies to observe the liquid flow pattern and thermal distributions [37–40]. The vorticity and energy equations are written as follows:

Vorticity equation

\[
\frac{\partial \omega}{\partial t} + \frac{\partial}{\partial x} \left( \omega \frac{\partial \psi}{\partial x} \right) - \frac{\partial}{\partial y} \left( \omega \frac{\partial \psi}{\partial y} \right) = \frac{\mu_{nf}}{\rho_{nf}} \left( \frac{\partial \omega}{\partial x^2} + \frac{\partial \omega}{\partial y^2} \right) + \frac{(\phi \rho_p \beta_\gamma + (1 - \phi) \rho_f \beta_\gamma)}{\rho_{nf}} \nabla \left( \frac{\partial T}{\partial x} \right)
\] (1)

Energy equation

\[
\frac{\partial T}{\partial t} + \frac{\partial}{\partial x} \left( \frac{\partial T}{\partial x} \right) - \frac{\partial}{\partial y} \left( \frac{\partial T}{\partial y} \right) = \frac{\rho_{nf}}{\rho_{nf}} \left( \frac{\partial \omega}{\partial x} + \frac{\partial \omega}{\partial y} \right)
\] (2)

The kinematics equation can be written as:

\[
\omega = -\left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right)
\] (3)

where the thermal diffusivity is calculated based on:

\[
\alpha_{nf} = \frac{k_{nf}}{(\rho c_p)_{nf}}
\] (4)

The effective density of main liquid with ultrafine solid particles described as:

\[
\rho_{nf} = (1 - \phi) \rho_f + \phi \rho_p
\] (5)

The details of all nanofluids and non-dimensional parameters can be found in [41].
Table 1. Comparison of the average Nusselt number along the hot wall (Pr = 0.7).

| Domain size | Ra  | Present work | Ref. [42] | Ref. [43] |
|-------------|-----|--------------|-----------|-----------|
| 100 × 100   | $10^4$ | 2.253        | 2.245     | 2.243     |
| 200 × 200   | $10^4$ | 2.248        | 2.245     | 2.243     |

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Fig 1. Comparison of the temperature at the mid-section (Y = 0.5) of the cavity by Khanafer et al. [2] (left) and the present results.

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Fig 2. Temperature and velocity profiles for the hot object in the square domain.

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Fig 3. Temperature and distribution at x = 0.5 and y = 0.5 for the hot object in the square domain.

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3. Results and discussion

For validation of this paper, the $Nu$ number in our study is compared with previous work. Table 1 shows a great agreement between the numerical results and existing data in the

![Velocity profile in vertical direction](https://doi.org/10.1371/journal.pone.0233850.g004)

![Velocity profile in horizontal direction](https://doi.org/10.1371/journal.pone.0233850.g005)

![Temperature and velocity profiles for three hot objects](https://doi.org/10.1371/journal.pone.0233850.g006)
literature for $Pr = 0.7$ and square shape domain. Additionally, the obtained results for $Ra = 10000$ are compared with literature and is perceived that our finding perfectly match with previous work (Fig 1). In this study, the analysis of the heating structure system and effect
of nanofluids on the temperature distribution are investigated. To start the analysis, a hot wall at the right, a cold wall at the left and the adiabatic walls on the top and bottom are added. In addition to the walls, the hot cylinder is added in the domain. In general, having a square

**Fig 10.** Effect of different amount of nanofluids on the thermal distribution.

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**Fig 11.** Effect of different amount of nanofluids on Nu number.

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shape domain provides the normal fluid and heat distribution, while by adding hot cylinder in the domain, we can change this distribution which affects the optimization of heating equipment. Fig 2 shows that adding the hot cylinder causes a high-temperature region on the top and bottom right, and the fluid velocity in the domain appears with a large vortex at the left of the domain. Moreover, the maximum heat transfer appears at the left side of the cylinder. Fig 3 shows the temperature profiles along the $y$ and $x$ axis at the middle of the domain as well as the $Nu$ number along with the hot wall. As the figure shows there is a low temperature at the bottom of the domain. As the position in $y$ direction increases, the temperature increases up to the maximum value. By getting close to the cylinder, $T$ is the maximum. However, after the cylinder area, almost near the adiabatic wall on the top, a small decrement in temperature is seen. Figs 4 and 5 show the velocity profile along the vertical and horizontal lines. As can be seen, due to having the vortex near the left wall, the positive and negative velocity representing the vortex area can be observed.
Fig 14. Effect of different amount of nanofluids on the velocity distribution.

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To explore the effect of the hot cylinder in this study, more cylinders are added in the domain. Adding more solid structure causes a very hot region in the domain and small vortex structure between objects (Fig 6 and Fig 7). Figs 8 and 9 illustrate the velocity profiles along the vertical and horizontal lines. The results show the small shape of the vortex in the domain due to having the multi-solid structure in the cavity.

After adding nanofluid into the system with only one cylindrical object, the fluid flow and heat distribution for the different amount of nanoparticles are able to be observed. Adding more particles in the main liquid causes higher heat transfer rate in the system. Fig 10 shows the effect of the amount of nanofluids on the thermal distribution. As the graph shows, by adding more nanoparticles into the system, more heat transfer rate is observed. Fig 11 shows the effect of nanofluids on the $Nu$ number. The higher amount of nanoparticles causes more uniform distribution in the square shape domain. In addition, the high amount of nanofluids has an effect on the vortex structure. The nanofluids result in smaller vortex domain compared with the low amount of nanoparticles (Fig 12).

Fig 13 shows the temperature distribution along the hot wall. The results show that the temperature is uniformly distributed along this wall. The amount of nanoparticles also decrease the velocity of the main liquids and generates very small vortex shape with lower maximum and minimum velocity compared with zero nanoparticle system (Fig 14).

4. Conclusions
Nanofluids have a significant effect on the improvement of thermal equipment in industries. This package of fluid-structure enables engineers and researchers to design and optimize a high heat transfer mechanism in the different processes, particularly heat exchanging systems. There is a need to use capable numerical methods in simulation of multi-solid walls without the usual limitation of numerical methods such as computational resources and stability of numerical methods in the complex multi-structure body. This study uses the CIP method for the prediction of multi-solid walls in the present of nanofluids in the system. The results show that the CIP method can accurately predict the nanofluid pattern and thermal distribution in the domain. Using multi-solid walls causes controlling the liquid vortex and change the thermal distribution. Additionally, adding nanoparticles in the main liquid results in higher heat transfer rates throughout the domain which increases the overall efficiency of the system. The main limitation of the current model is computing time in a large domain of simulation and coupling mechanistic models to CIP computing nodes. Additionally, calculation of turbulence spectrum, eddy structure and velocity distribution for high Reynolds number can be challenging in the domain, particularly when forcing flow such as shear flow is a main forcing scheme. To solve the computing time, the model can be written in the parallel cluster nodes, and with correct transferring information through boundaries, the computational time significantly decreases. The main suggestion for coupling mechanistic models (such as chemical reactions and deformation of lagrangian particles) in every calculation, CIP computing nodes can transfer fluid flow and thermal information into the mechanistic model. Then in every physical time we can see rate of chemical reactions or particle deformation and dynamics. For calculation of turbulence flow, Large Eddy Simulation (LES) is suggested to resolve more eddy and vortex structure in the domain. However, this method of calculation can be time consuming for large domain.

Author Contributions

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References

1. Xuan Y, Li Q. Heat transfer enhancement of nanofluids. IJHFF. 2000; 21(1):58–64.
2. Mohammed H, Al-Aswadi A, Shuaib N, Saidur R. Convective heat transfer and fluid flow study over a step using nanofluids: a review. Renewable and Sustainable Energy Reviews. 2011; 15(6):2921–39.
3. Daungthongsuk W, Wongwises S. A critical review of convective heat transfer of nanofluids. Renewable and sustainable energy reviews. 2007; 11(5):797–817.
4. Abu-Nada E. Effects of variable viscosity and thermal conductivity of Al2O3–water nanofluid on heat transfer enhancement in natural convection. International Journal of Heat and Fluid Flow. 2009; 30(4):679–90.
5. Dagtekin I, Oztop HF, Bahloul A. Entropy generation for natural convection in Γ-shaped enclosures. International Communications in Heat and Mass Transfer. 2007; 34(4):502–10.
6. Nakhjiri AT, Heydarinasab A, Bakhtiar O, Mohammadi T. Modeling and simulation of CO2 separation from CO2/CH4 gaseous mixture using potassium glycinate, potassium arginine and sodium hydroxide liquid absorbents in the hollow fiber membrane contactor. Journal of Environmental Chemical Engineering. 2018; 6(1):1500–11.
7. Nakhjiri AT, Heydarinasab A, Bakhtiar O, Mohammadi T. Experimental investigation and mathematical modeling of CO2 sequestration from CO2/CH4 gaseous mixture using MEA and TEA aqueous absorbents through polypropylene hollow fiber membrane contactor. J Membr Sci. 2018; 565:1–13.
8. Shirazian S, Moghadass A, Moradi S. Numerical simulation of mass transfer in gas–liquid hollow fiber membrane contactors for laminar flow conditions. Simulation Modelling Practice and Theory. 2009; 17(4):708–18.
9. Shirazian S, Marjani A, Rezakazemi M. Separation of CO2 by single and mixed aqueous amine solvents in membrane contactors: fluid flow and mass transfer modeling. Engineering with Computers. 2012; 28(2):189–98.
10. Nakhjiri AT, Heydarinasab A. Computational simulation and theoretical modeling of CO2 separation using EDA, PZEA and PS absorbents inside the hollow fiber membrane contactor. Journal of Industrial and Engineering Chemistry. 2019; 78:106–15.
11. Ding Y, Chen H, Wang L, Yang C-Y, He Y, Yang W, et al. Heat transfer intensification using nanofluids. KONA Powder and Particle Journal. 2007; 25:23–38.
12. Nabavitabatabayi M, Shirani E, Rahimian MH. Investigation of heat transfer enhancement in an enclosure filled with nanofluids using multiple relaxation time lattice Boltzmann modeling. International Communications in Heat and Mass Transfer. 2011; 38(1):128–38.
13. Xuan Y, Yao Z. Lattice Boltzmann model for nanofluids. Heat and mass transfer. 2005; 41(3):199–205.
14. He Y, Qi C, Hu Y, Qin B, Li F, Ding Y. Lattice Boltzmann simulation of alumina-water nanofluid in a square cavity. Nanoscale research letters. 2011; 6(1):184. https://doi.org/10.1186/1556-276X-6-184 PMID: 21711683
15. Nemati H, Farhadi M, Sedighi K, Fattahi E, Darzi A. Lattice Boltzmann simulation of nanofluid in lid-driven cavity. International Communications in Heat and Mass Transfer. 2010; 37(10):1528–34.
16. Bararnia H, Soleimani S, Ganji D. Lattice Boltzmann simulation of natural convection around a horizontal elliptic cylinder inside a square enclosure. International Communications in Heat and Mass Transfer. 2011; 38(10):1436–42.
17. Fattahi E, Farhadi M, Sedighi K, Nemati H. Lattice Boltzmann simulation of natural convection heat transfer in nanofluids. International Journal of Thermal Sciences. 2012; 52:137–44.
18. Lai F-H, Yang Y-T. Lattice Boltzmann simulation of natural convection heat transfer of Al2O3/water nanofluids in a square enclosure. International journal of thermal sciences. 2011; 50(10):1930–41.
19. Kefayati G, Hosseinizadeh S, Gorji M, Sajjadi H. Lattice Boltzmann simulation of natural convection in an open enclosure subjugated to water/copper nanofluid. International Journal of Thermal Sciences. 2012; 52:91–101.

20. Kefayati GR, Hosseinizadeh S, Gorji M, Sajjadi H. Lattice Boltzmann simulation of natural convection in tall enclosures using water/SiO2 nanofluid. International Communications in Heat and Mass Transfer. 2011; 38(6):798–805.

21. Zhou L, Xuan Y, Li Q. Multiscale simulation of flow and heat transfer of nanofluid with lattice Boltzmann method. International Journal of Multiphase Flow. 2010; 36(5):364–74.

22. Khodadadi J, Hosseinizadeh S. Nanoparticle-enhanced phase change materials (NEPCM) with great potential for improved thermal energy storage. ICHMT. 2007; 34(5):534–43.

23. Schmid G. Nanoparticles: from theory to application: John Wiley & Sons; 2011.

24. Khodadadi J. Nanoparticle-enhanced Phase Change Materials (NePCM) and HRD. Univ. of Alabama, Tuscaloosa, AL (United States), 2013.

25. Aydin O, Yang W-J. Natural convection in enclosures with localized heating from below and symmetrical cooling from sides. International Journal of Numerical Methods for Heat & Fluid Flow. 2000; 10(5):518–29.

26. Das S, Morsi Y. Natural convection inside dome shaped enclosures. International Journal of Numerical Methods for Heat & Fluid Flow. 2002; 12(2):126–41.

27. Sebti S, Khallary S, Mirzaee I, Hosseinizadeh S, Kashani S, Abdollahzadeh M. A numerical investigation of solidification in horizontal concentric annuli filled with nano-enhanced phase change material (NEPCM). World Applied Sciences Journal. 2011; 13(1):9–15.

28. Delavar MA, Farhadi M, Sedighi K. Numerical simulation of direct methanol fuel cells using lattice Boltzmann method. International journal of hydrogen energy. 2010; 35(17):9306–17.

29. Mahmoodi M. Numerical simulation of free convection of a nanofluid in L-shaped cavities. International Journal of Thermal Sciences. 2011; 50(9):1731–40.

30. Yan Y, Zu Y. Numerical simulation of heat transfer and fluid flow past a rotating isothermal cylinder—a LBM approach. International Journal of Heat and Mass Transfer. 2008; 51(9–10):2519–36.

31. Fard MH, Esfahany MN, Talaei M. Numerical study of convective heat transfer of nanofluids in a circular tube two-phase model versus single-phase model. International Communications in Heat and Mass Transfer. 2010; 37(1):91–7.

32. Eastman JA, Choi U, Li S, Thompson L, Lee S. Enhanced thermal conductivity through the development of nanofluids. MRS online proceedings library archive. 1996;457.

33. Tahery A, Pesteie S, Zehoorooch A. Numerical study of heat transfer performance of homogenous nanofluids under natural convection. International Journal of Chemical Engineering and Applications. 2010; 1(1):49.

34. Oztop HF, Abu-Nada E. Numerical study of natural convection in partially heated rectangular enclosures filled with nanofluids. International journal of heat and fluid flow. 2008; 29(5):1326–36.

35. Wang X-Q, Mujumdar AS. A review on nanofluids-part I: theoretical and numerical investigations. Brazilian Journal of Chemical Engineering. 2008; 25(4):613–30.

36. Shi Y, Zhao T, Guo Z. Thermal lattice Bhatnagar-Gross-Krook model for flows with viscous heat dissipation in the incompressible limit. Physical Review E. 2004; 70(6):066310.

37. Sheldareh A, Safdari A, Pourtousi M, Sidik N. Prediction of particle dynamics in lid-driven cavity flow. International Review on Modelling and Simulations. 2012; 5(3).

38. Pourtousi M, Sidik NAC, Safdari A, Khan AA. MULTI-RELAXATION TIME LATTICE BOLTZMANN SIMULATION FOR INCOMPRESSIBLE FLUID FLOW. Jurnal Mekanikal. 2012; 35(2).

39. Pourtousi M. Simulation of Particle Motion in Incompressible Fluid by Lattice Boltzmann MRT Model: Universiti Teknologi Malaysia; 2012.

40. Azwadi C, Razzaghian M, Pourtousi M, Safdari A. Numerical prediction of free convection in an open ended enclosure using lattice Boltzmann numerical method. Int J Mech Mater Eng. 2013; 8:58–62.

41. Safdari A, Dabir H, Kim KC. Cubic-Interpolated Pseudo-particle model to predict thermal behavior of a nanofluid. Computers & Fluids. 2018; 164:102–13.

42. Khanafer K, Vafai K, Lightstone M. Buoyancy-driven heat transfer enhancement in a two-dimensional enclosure utilizing nanofluids. ICHMT. 2003; 46(19):3639–53.

43. Davis DV. Natural convection of air in a square cavity; A benchmark solution. Int J Numer Meth Fluids. 1983(3):249–64