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# Mathematical Modeling for Nanofluids Simulation: A Review of the Latest Works

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## Abstract

Exploiting nanofluids in thermal systems is growing day by day. Nanofluids having ultrafine solid particles promise new working fluids for application in energy devices. Many studies have been conducted on thermophysical properties as well as heat and fluid flow characteristics of nanofluids in various systems to discover their advantages compared to conventional working fluids. The main aim of this study is to present the latest developments and progress in the mathematical modeling of nanofluids flow. For this purpose, a comprehensive review of different nanofluid computational fluid dynamics (CFD) approaches is carried out. This study provides detailed information about the commonly used formulations as well as techniques for mathematical modeling of nanofluids. In addition, advantages and disadvantages of each method are rendered to find the most appropriate approach, which can give valid results.

**Keywords:** nanofluid, CFD, numerical simulation, mathematical modeling, single- and two-phase methods

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## 1. Introduction

In general, the assessment of the thermal performance of a system through numerical simulations is much affordable compared to experimental studies with high expenses of material and

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equipment. The significance of a numerical study is highlighted when a nanofluid is utilized as the working fluid. High costs for the production of nanofluids and difficulties in preparing stable nanofluids are the main barriers to perform experiments with nanofluids. Therefore, numerical modeling of nanofluids, where a suitable approach is selected to simulate the flow, could be the best solution for problems involved with nanoparticle suspensions.

However, in spite of considerable developments in computing power and methods, literature review reveals that there is no comprehensive study to conclude the best technique for the modeling of nanofluids. In particular, due to the ultrafine size of nanoparticles, the governing terms in multiphase models are still not entirely identified. In the present work, latest studies on numerical simulations of nanofluid flow are reviewed with a particular focus on different multiphase schemes.

## 2. Numerical methods for nanofluids' flow simulation

Nanofluid computational fluid dynamic (CFD) modeling can be classified into two main groups: single-phase and two-phase models. However, there are few other models that may not be included in these categories, such as Lattice-Boltzmann method (LBM). Moreover, different numerical approaches have been employed to solve models mentioned above to predict thermal and hydraulic characteristics of nanofluids flow. Finite volume method (FVM) and finite element method (FEM) are two main approaches for solving the governing equations of nanofluid problems. However, finite difference method (FDM), control volume-based finite element method, and some novel numerical approaches such as homotopy analysis method (HAM) and smoothed particle hydrodynamics (SPH) methods have also been utilized in the previous studies. In this study, a comprehensive review of various numerical methods for the simulation of nanofluids is accomplished.

### 2.1. Single-phase approaches

Although suspension of a nanofluid is inherently a two-phase fluid, if some proper assumptions are made, it can be considered as a homogeneous liquid. Due to the existence of ultrafine nanoparticles, it is assumed that these particles can be easily dispersed in the host fluid. For this purpose, both the nanoparticles and base fluid are considered to be in thermal balance without any slip between their molecules. Therefore, under such assumptions, in many studies, nanofluids have been assumed as a single-phase fluid.

#### 2.1.1. Conventional single-phase model

Mass, momentum, and energy equations, which are used for conventional liquids, could also be applied to single-phase flow with the above assumptions. In this case, only thermophysical properties of nanofluids should be determined. Therefore, the governing equations in the steady state can be expressed as below [1]:

Conservation of mass:

$$\nabla \cdot (\rho_{eff} \vec{u}) = 0 \quad (1)$$

Conservation of momentum:

$$\nabla \cdot (\rho_{eff} \vec{u} \vec{u}) = -\nabla P + \nabla \cdot (\mu_{eff} \nabla \vec{u}) - (\rho\beta)_{eff} (T - T_0) g \quad (2)$$

Conservation of energy:

$$\nabla \cdot ((\rho c_p)_{eff} \vec{u} T) = \nabla \cdot (k_{eff} \nabla T) \quad (3)$$

There are numerous publications simulating nanofluids characteristics as a single-phase fluid. Mixed convection heat transfer in a T-shaped lid-driven cavity was examined numerically by Mojumder et al. [2]. A residual FEM model was applied for the numerical simulation. They validated their simulation code against data of Abu-Nada, Chamkha [3]. The results revealed that higher Grashof number causes rise in the heat transfer rate.

Turbulent nanofluid flow for different nanoparticles such as alumina, cupric oxide, and titania was investigated by Rostamani et al. [4] at various concentrations in a long horizontal duct under constant heat flux. They employed the control volume approach and temperature-dependent thermophysical properties. It was found that increasing the number of dispersed nanoparticles in base fluid increases the pumping power and heat transfer rate. In addition, the predicted Nusselt numbers in some cases demonstrated good agreements to the obtained results by Pak, Cho [5], and Maiga et al. [6] correlations.

Abu-Nada [7] considered the Rayleigh-Benard-free convection heat transfer in CuO-water nanofluids using FVM, where the effect of temperature-dependent properties was the primary objective. The obtained results by temperature-dependent models were also compared with classic models (Maxwell-Garnett (MG) and Brinkman). Results displayed that for  $Ra > 10^3$ , the effect of temperature on fluid flow and heat transfer was insignificant due to the presence of high viscosity, which was caused by the nanoparticles volume fraction.

Bouhaleb and Abbassi [8] employed Control Volume-Finite Element method to study the free convection in an inclined cavity. They solved the free convection problem using Boussinesq approximation and employing the SIMPLER algorithm for velocity-pressure coupling. The results showed that the variation of inclination angel highlights a hysteresis behavior of the nanofluid flow. Also, increasing the diameter of solid nanoparticles led to a strong decay in heat transfer. Furthermore, they concluded that the efficiency of heat transfer strongly depends on the diameter of nanoparticles, not its concentration in base fluid.

While a considerable number of recent studies on numerical simulation of nanofluids have been employed by FVM [9–11] and FEM [12–14] for their studies, in several studies Finite Difference Method has been used for different applications of nanofluids. For instance, Buddakkagari and Kumar [15] studied laminar-forced convection of a nanofluid over a vertical

cone/plate. The non-dimensional governing equations were solved using FDM model, Crank-Nicolson type. The results illustrated that the Prandtl number affects the boundary layer dramatically. Furthermore, the momentum boundary layer was more affected by higher values of Lewis number. Finally, it was concluded that the boundary layer growth depends on Brownian motion and thermophoresis force.

However, applying the single-phase model for nanofluids has some limitations. For instance, the results obtained from this model were strongly dependent on adopted thermophysical properties and in some cases using the single-phase model may underestimate the Nusselt number, compared to models adopting temperature-dependent properties [16, 17]. The reason behind this could be due to various factors such as gravity, friction forces, Brownian motion, and solid/liquid interface. Ding and Wen [18] showed that the primary assumption of homogeneous fluid is not always acceptable. However, the review of the previous works illustrates that choosing the appropriate thermophysical property correlations in the single-phase method results in a reasonable estimation of nanofluids properties [19, 20]. Therefore, selecting suitable thermophysical properties such as variable properties, and considering the chaotic movement of nanoparticles (dispersion model) may compensate, to some extent, the limitations of single-phase model.

### 2.1.2. Thermal dispersion model

Brownian and gravity forces, the friction force between the base fluid and nanoparticles, sedimentation, and dispersion may coexist in a nanofluid flow. In fact, slip motion between liquid molecules and solid particles is not negligible, and the random movement of nanoparticles ameliorates the thermal dispersion in nanofluids, which reinforces heat transfer. For the first time, the thermal dispersion model was suggested by Xuan and Roetzel [21]. They assumed that nanoparticles move randomly, causing small chaos in velocity and temperature magnitudes ( $T'$  and  $\vec{u}'$ ). The essential phase averages can be written as [21]:

$$T = \langle T \rangle^f + T' \quad (4)$$

$$\vec{u} = \langle \vec{u} \rangle^f + \vec{u}' \quad (5)$$

where

$$\langle T \rangle^f = \frac{1}{V_f} \int_{V_f} T dV \quad (6)$$

$$\langle \vec{u} \rangle^f = \frac{1}{V_f} \int_{V_f} \vec{u} dV \quad (7)$$

$$\frac{1}{V_f} \int_{V_f} T' dV = 0 \quad (8)$$

By assuming that the boundary layer between the liquid and solid phases is negligible, unsteady-state, energy equation can be written as

$$(\rho c_p)_{nf} \left[ \frac{\partial \langle T \rangle^f}{\partial t} + \langle \vec{u} \rangle^f \cdot \nabla \langle T \rangle^f \right] = \nabla \cdot (k_{nf} \nabla \langle T \rangle^f) - (\rho c_p)_{nf} \nabla \cdot \langle \vec{u} T' \rangle^f \quad (9)$$

The thermal dispersion generates a heat flux in the flow that is equal to

$$q_d = (\rho c_p)_{nf} \langle \vec{u} T' \rangle^f = -k_d \cdot \nabla \langle T \rangle^f \quad (10)$$

$k_d$  is the thermal conductivity tensor due to dispersion. Now, Eq. (9) can be rewritten as

$$\frac{\partial \langle T \rangle^f}{\partial t} + \langle \vec{u} \rangle^f \cdot \nabla \langle T \rangle^f = \nabla \cdot \left[ (\alpha_{nf} \mathbf{I} + \frac{\mathbf{k}_d}{(\rho c_p)_{nf}}) \cdot \nabla \langle T \rangle^f \right] \quad (11)$$

where  $\alpha$  is the thermal diffusivity and  $\mathbf{I}$  is the identity tensor. The following form may be applicable for the effective thermal conductivity of nanofluid:

$$k_{eff} = k_{nf} + k_d \quad (12)$$

where  $k_d$  refers to the dispersed thermal conductivity coefficient. Despite the fact that this term plays a key role in dispersion model, just a few correlations were proposed in the literature. Xuan and Roetzel [21] with reference to some publications in porous media [22, 23] proposed the following forms:

$$k_d = C^* (\rho c_p)_{nf} u R, \quad k_d = C_d (\rho c_p)_{nf} u R d_p \phi \quad (13)$$

$C_d$  is an unknown constant and  $R$  is referred to pipe radius. Khaled and Vafai [24] investigated heat transfer enhancement by considering dispersion effects. They used the following linearized model introduced by Xuan and Roetzel [21] correlations for dispersed thermal conductivity of nanofluids:

$$k_d = C^* (\rho c_p)_{nf} \phi H u_m \quad (14)$$

where  $H$  is the half of duct height,  $u_m$  is the average bulk velocity, and  $C^*$  is an unknown constant. By employing control volume approach, Mojarrad et al. [25] analyzed the heat transfer of  $\alpha$ -alumina-water nanofluid in the entrance region of a rounded pipe. They also compared their results with experimental data. The results showed that dispersion model provides reasonable outcomes in spite of its simplicity. Moreover, they suggested a new correlation for radial dispersed thermal conductivity:

$$k_d = C_d (\rho c_p)_{nf} \frac{R\phi}{d_p} \left( \frac{\partial T}{\partial r} \right) \quad (15)$$

By using dispersion model, Zeinali Heris et al. [26, 27] investigated convective heat transfer of different nanofluids. They studied heat transfer augmentation due to nanofluids flow through the tubes with different cross-section geometries. The numerical results were validated against experimental data [28, 29] and good agreement was observed. The results showed that the Nusselt number would enhance with increasing particle loading and decreasing particle size.

Thermal behavior of nanofluids in a cavity was analyzed by Kumar et al. [30]. The dimensionless-governing equations were resolved via semi-explicit FVM solver. The Grashof number, volume concentration, and nanoparticles shape effects on heat transfer rate were assessed. The results showed that the dispersed thermal conductivity is more intensive in the vicinity of walls in comparison with pipe center. Also, it was found that dispersed thermal conductivity and hydraulic diameter of the particles are strongly dependent to each other.

Akbaridoust et al. [31] examined laminar steady-state nanofluid flow through helically shaped tubes, both numerically and experimentally. The governing equations in three-dimensional (3-D) form were solved by finite difference approach, using a FORTRAN code. Dispersion model was modified in order to be applicable for helical tubes. This modification resulted in minimized difference between numerical results and experimental data. The results showed that higher curvature ratios cause more heat transfer rates.

## 2.2. Two-phase approaches

Due to some factors such as Brownian force, Brownian diffusion, friction force, thermophoresis, and gravity, nanofluids may be considered two-phase fluids by nature. Therefore, the classic theory of solid-liquid mixture can be applied to nanofluids. In such models, nanoparticles and base fluid are considered as two separate phases with different temperatures and velocities. Although two-phase approaches may obtain realistic results, they have high computational cost in comparison to single-phase models. Two-phase approaches can be categorized into two general models: Lagrangian-Eulerian and Eulerian-Eulerian.



### 2.2.1. Lagrangian-Eulerian model

In the Lagrangian-Eulerian or discrete phase model, the fluid phase is considered as a continuum by solving the N-S equations in time-averaged form, while the dispersed phase was solved by tracking the particles in the Lagrangian frame. Also, in this model, the interaction between fluid and particles presented as a source term in both momentum and energy equations.

Mathematical formulations of the Lagrangian-Eulerian in two-phase model can be written as follows [32]:

Conservation of mass:

$$\nabla \cdot (\rho \vec{u}) = 0 \quad (16)$$

Conservation of momentum:

$$\nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla P + \nabla \cdot (\mu \nabla \vec{u}) + S_m \quad (17)$$

Conservation of energy:

$$\nabla \cdot (\rho c_p \vec{u} T) = \nabla \cdot (k \nabla T) + S_e \quad (18)$$

where  $S_m$  and  $S_e$  are source/sink terms representing the exchange of momentum and energy between liquid and solid phases. The momentum and energy source/sink terms are defined as [33, 34]

$$s_m = \frac{1}{\delta V} \sum_{np} \vec{F} \quad (19)$$

$$s_e = \frac{1}{\delta V} \sum_{np} Nu_p \pi d_p k_p (T - T_p) \quad (20)$$

where  $Nu_p$  can be computed from the Ranz correlation [35]:

$$Nu_p = 2 + 0.6 Re_p^{0.5} Pr^{0.333} \quad (21)$$

In Lagrangian reference frame, the particle motion and energy equations are as follows:



$$m_p \frac{d\vec{u}_p}{dt} = \vec{F}_g + \vec{F}_D + \vec{F}_L + \vec{F}_{Br} + \vec{F}_b \quad (22)$$

$$m_p c_p \frac{dT_p}{dt} = Nu_p \pi d_p k_f (T_f - T_p) \quad (23)$$

In Eq. (22),  $F$  stands for various forces including gravity, drag, Saffman's lift, Brownian, and buoyancy, respectively.

Turbulent nanofluid flow in helical tubes was investigated numerically and experimentally by Bahremand et al. [36]. The numerical simulation was performed by both single-phase model and Lagrangian-Eulerian approach in connection with renormalization group (RNG)  $k-\varepsilon$  model. ANSYS CFX software was used for solving the governing equations. The results indicated that nanofluids with a higher concentration exhibit a greater heat transfer coefficient and pressure drop. Also, it was found that the two-phase model yields more accurate results compared to single-phase model.

Alumina-water nanofluid flow and heat transfer in a long tube with uniform heating at the walls were investigated by Moraveji and Esmaeili [37]. The simulations were conducted in both single- and two-phase methods where the governing equations were solved by FVM. Both temperature-dependent and constant thermophysical properties were considered in the study. The results of the modeling revealed that the temperature-dependent properties are more sensitive to the Reynolds number variations and led to higher values of the Nusselt number. Comparison between single-phase and two-phase (discrete phase) models showed the maximum difference of 11% for the average heat transfer coefficient.

Tahir and Mital [38] studied the laminar-forced convection of  $Al_2O_3$ -water nanofluid in a tube numerically. They analyzed the impacts of the Reynolds number, particle diameter, and volume fraction of the particles in their study. A good agreement was achieved between the simulation and experimental data using discrete phase method. The results of the survey demonstrated that the heat transfer coefficient increased linearly with both the Reynolds number and volume fraction of nanoparticles. However, there was a non-linear parabolic decrease with increasing nanoparticle size. It was concluded that the Reynolds number and volume fraction have the maximum and the minimum effects on heat transfer coefficient, respectively.

A comprehensive simulation of turbulent-forced convection for Cu-water was carried out by Behroyan et al. [39]. The Reynolds number of the flow was chosen between 10,000 and 25,000, where the volume fraction of copper nanoparticles was taken in the range of 0.0–2.0%. Two single-phase models (Newtonian and non-Newtonian) and three two-phase models were employed in this study. The ANSYS commercial CFD package was utilized to solve the governing equations. The obtained results showed that the Newtonian single-phase method as well as discrete phase method is in better agreement with experimental data, compared to other numerical approaches.

The present literature survey reveals that using Lagrangian-Eulerian approach for modeling the heat transfer of nanofluids is in early stages. Therefore, more studies are required to be conducted to determine the capability of the Lagrangian-Eulerian model, especially in turbulent regime [40]. Also, in some other studies such as Safaei et al. [32] and Xu et al. [41], it is emphasized that Lagrangian-Eulerian is a suitable model just for low concentration two-phase suspensions ( $\varphi < 1\%$ ). Moreover, it was mentioned that this model needs extremely high computational time due to a large amount of calculation.

### 2.2.2. Eulerian-Eulerian model

The other important branch of two-phase models is the Eulerian-Eulerian model. Since the Eulerian-Eulerian model is suitable for mixtures with a high amount of particles, applying this model to nanofluids consisting of an extremely large number of nanoparticles is recommended. The main models of Eulerian-Eulerian available in the literature are three models including Mixture, Eulerian, and VOF (volume of fluid).

#### 2.2.2.1. Volume of fluid model

In the VOF model, the volume fractions of all phases are obtained for the entire domain of study, by solving the continuity equation for the secondary phases. A single set of momentum equations is solved for all the phases to find the velocity components. The sum of all employed phases' volume fractions is equal to unity. Accordingly, the primary phase volume fraction magnitude is achieved. In addition, all the physical properties are calculated by using an average weighted of different phases according to their volume fraction on each control volume. Finally, a shared temperature is calculated from a single energy equation [42].

Mass conservation for VOF model can be expressed as

$$\nabla \cdot (\varphi_z \rho_z \vec{u}_z) = 0 \quad (24)$$

where  $\sum_{z=1}^n \varphi_z = 1$  and all properties are computed such as  $N = \sum_{z=1}^n \varphi_z N_z$ .

In this model, Eqs. (2) and (3) are used as momentum and energy equations.

According to literature, a few studies have been done on using the VOF model for the simulation of nanofluids. Akbari et al. [43] studied turbulent-forced convective heat transfer of  $\text{Al}_2\text{O}_3$ -water as well as Cu-water nanofluids inside a horizontal tube under uniform heat flux. The governing equations were solved implementing different numerical approaches, for example, single-phase, VOF, mixture, and Eulerian models, using FLUENT software. The results showed that the thermal field forecasting by multiphase models was different from the results of experimental data and single-phase approach. However, single-phase and two-phase models predicted almost same hydrodynamic results. It was concluded that unlike the results of previous studies [17, 44], two-phase models overestimate the thermal field. Under similar conditions, however, Hejazian et al. [45] found different results when investigating the

turbulent convection of  $\text{TiO}_2$ -water nanofluid in a horizontal tube using FVM method. The results of this study showed that the mixture and VOF models are more appropriate to predict the heat transfer field, compared to single-phase model.

Turbulent heat transfer of nanofluids flow through a mini-channel heat sink was analyzed by Naphon and Nakharintr [46]. The  $k$ - $\epsilon$  turbulence model with single-phase, mixture, and VOF approaches was employed to analyze the heat transfer and flow characteristics. Also, some experiments conducted to verify the predicted results and reasonable agreements were achieved. It was concluded that the single-phase model cannot predict the Nusselt number with accuracy as good as mixture and VOF models because the impacts of Brownian motion and non-uniform distribution of nano-particles in the solution domain are not considered in the single-phase model. In addition, under similar conditions, VOF and mixture models present more appropriate results compared to the single-phase model.

Hanafizadeh et al. [47] carried out a study to compare single and two-phase approaches for  $\text{Fe}_3\text{O}_4$ -water nanofluid in both developing and fully developed regions in a circular tube under constant heat flux. The study was conducted for 0.5–2 vol. % and  $300 \leq \text{Re} \leq 1200$ . The results showed that higher values of both Reynolds number and volume fraction would augment the average heat transfer coefficient, while just increasing the number of dispersed nanoparticles does not have a considerable impact on heat transfer enhancement. Also, in the fully developed region, a higher number of dispersed nanoparticles in base fluid would reduce the error of studied numerical methods. On the other hand, in developing region of a tube and for low Reynolds numbers, increase in nanofluid volume fraction would decrease the accuracy of numerical methods, while this trend was reversed for moderate and high Reynolds numbers.

In total, since a limited number of studies have used this numerical approach, further studies are needed to evaluate the capability of the VOF model.

#### 2.2.2.2. Mixture model

The mixture model is one of the most popular methods for modeling of multiphase slurry flows. The main feature of this approach is that only one set of velocity elements is solved for the mixture momentum conservation equations. The velocities of dispersed phases are extracted from the algebraic formulations [48]. Moreover, since the primary phase affects the secondary phase through drag force and turbulence, the effect of secondary phase on the primary phase could be found through mean momentum reduction and turbulence. The basic assumptions of mixture model are as follows [49, 50]:

- All phases share a single pressure.
- The interaction between different dispersed phases is assumed to be negligible.
- Nanoparticles in the secondarily dispersed phase are spherical in shape, with a uniform size.
- The concentration of the secondarily dispersed phases is solved by a scalar equation, considering the correction made by phase slip.

The governing equations of the nanofluids' mixture model can be written as follows [51]:

Continuity:

$$\frac{\partial}{\partial t}(\rho_m) + \nabla \cdot (\rho_m \vec{u}_m) = 0 \quad (25)$$

where

$$\vec{u}_m = \frac{\sum_{Z=1}^n \varphi_Z \rho_Z \vec{u}_Z}{\rho_m} = \vec{u}_Z \quad (26)$$

and

$$\rho_m = \sum_{Z=1}^n \varphi_Z \rho_Z \quad (27)$$

Momentum:

$$\frac{\partial}{\partial t}(\rho_m \vec{u}_m) + \nabla \cdot (\rho_m \vec{u}_m \vec{u}_m) = -\nabla P_m + \nabla \cdot [\mu_m (\nabla \vec{u}_m + \nabla \vec{u}_m^T)] + \rho_m \beta_m (T - T_0) g \quad (28)$$

where

$$\mu_m = \sum_{Z=1}^n \varphi_Z \mu_Z \quad (29)$$

Energy:

$$\frac{\partial}{\partial t} \rho_m h_m + \nabla \cdot (\rho_m h_m \vec{u}_m) + \nabla \cdot (P \vec{u}_m) = \nabla \cdot (k_m \nabla T) \quad (30)$$

where

$$\rho_m h_m = \sum_{Z=1}^n (\varphi_Z \rho_Z h_Z) \quad (31)$$

and

$$k_m = \sum_{Z=1}^n \phi_Z (k_Z) \quad (32)$$

As a pioneer, Behzadmehr et al. [44] employed single-phase approach as well as two-phase mixture model to study the turbulent heat transfer of copper-water nanofluid inside a circular tube. The results of their study revealed that the obtained results from mixture model are much closer to experimental data, compared to the results of single-phase model. In a similar study, Bianco et al. [52] analyzed the steady-state turbulent convection heat transfer of  $\text{Al}_2\text{O}_3$ -water nanofluid in a circular tube under constant heat flux. FLUENT commercial software was used to solve the governing equations. The results showed that single-phase and mixture models give approximately the same results at low concentrations (i.e.,  $\phi = 1\%$ ), while for higher concentrations, the difference between two models is considerable.

Shariat et al. simulated alumina-water nanofluid in an elliptic tube [53]. The impacts of nanoparticles mean diameter and buoyancy force on the nanofluid flow behaviors were investigated in that study. The three-dimensional equations of the mixture model were solved by using FVM. The results showed that at a specified value of Reynolds and Richardson numbers, an increase in nanoparticles size diminishes the Nusselt number while it does not have a remarkable effect on the friction factor. A non-linear relation between the nanoparticles size and heat transfer characteristics of nanofluid was also observed.

Laminar-free convection heat transfer of alumina-water nanofluid inside a cavity was studied by Corcione et al. [54]. The governing equations were solved by a CFD code based on a two-phase mixture model. Temperature-dependent effective properties considering the Brownian motion and thermophoresis were employed and different nanoparticles volume fractions were analyzed. It was found that the heat transfer trend reached a peak value at maximum particle loading. Using these results, new correlations were developed for different parameters such as the optimal particle loading and a maximum value of the heat transfer augmentation.

Goodarzi et al. [51] investigated both laminar and turbulent mixed convection of Cu-water nanofluid inside a rectangular shallow cavity. The upper movable lid of the cavity was considered at a lower temperature, compared to the bottom wall. FLUENT commercial code was utilized to solve the problem, along with some modifications in governing equations by developing user-defined function (UDF) codes. The results showed that the impact of the volume fraction on turbulent kinetic energy, turbulence intensity, skin friction, and wall shear stress is insignificant. However, under similar conditions, lower Richardson number leads to higher wall shear stress and turbulence kinetics energy.

The single- and two-phase models were employed by Naphon and Nakharintr [55] to investigate the 3-D laminar convection heat transfer of nanofluids inside a mini-channel heat sink. Some experiments were also carried out for validation purpose. The research outcomes demonstrated that two-phase mixture model is in better agreement with experimental results, compared to single-phase model.

Recently, Siavashi et al. [56] investigated the application of nanofluids and porous media to enhance the heat transfer inside an annular pipe. The simulation was conducted to investigate the effects of different parameters such as the Darcy and Reynolds numbers as well as porous medium radius and its position on heat transfer enhancement, heat loss, and entropy generation. Two-phase mixture model along with Darcy-Brinkman-Forchheimer equation was employed for nanofluid flow simulation in porous media. A FVM code was developed to solve the governing equations. The results showed that the geometry, nanoparticle concentration, and magnitude of the Reynolds number have considerable effects on both the performance and entropy generation numbers.

By reviewing the literature, it can be seen that among different multiphase approaches, the mixture model is the most popular model for nanofluids modeling. This popularity can be due to some facts such as accuracy, simplicity in both theory and implementation, and low computational cost. However, for using this model there are some limitations and requirements, which were addressed in detail by Moraveji and Ardehali [49], Bahiraei [50], and Goodarzi et al. [51].

#### 2.2.2.3. Eulerian model

In this model, pressure is assumed to be equal for all the phases, while other governing equations are solved separately for primary and secondary phases. The volume of the two phases is estimated by integrating the volume fraction on solution domain, where the aggregate of volume fractions totality becomes one [50]. The Eulerian model corresponding equations can be expressed as follows [42]:

Continuity:

$$\nabla \cdot (\varphi_z \rho_z \vec{u}_z) = 0 \quad (33)$$

where  $\vec{u}_z = \int_V \varphi_z dv$ ,  $\sum_{z=1}^n \varphi_z = 1$ .

Conservation of momentum ( $z^{\text{th}}$  phase):

$$\nabla \cdot (\varphi_z \rho_z \vec{u}_z \vec{u}_z) = \sum_{p=1}^n \vec{R}_{pz} + F_{\text{lift}_z} + \varphi_z \nabla \cdot (\mu_z \nabla \vec{u}) + \varphi_z \rho_z \vec{g} - \varphi_z \nabla P \quad (34)$$

where  $\sum_{p=1}^n \vec{R}_{pz} = \sum_{p=1}^n S_{pz} (\vec{u}_p - \vec{u}_z)$  denotes the interaction force between phases,  $S_{pz} = (\varphi_z \varphi_p \rho_z f) / \tau_p$ ,  $\tau_p = (\rho_p d_p^2) / (18 \mu_z)$ , and  $f$  indicates the drag friction, which is computed by Schiller and Naumann [57] recommendation:



$$f = \frac{C_D Re_p}{24} \quad (35)$$

where

$$C_D = \begin{cases} \frac{24(1 + 0.15 Re_p^{0.687})}{Re_p} & Re \leq 1000 \\ 0.44 & Re > 1000 \end{cases} \quad (36)$$

The nanoparticle Reynolds number ( $Re_p$ ) in Eq. (36) and lift force in Eq. (34) [58] are, however, based on particle-fluid relative velocity, which is extremely small for nanoparticles.

$$Re_p = \frac{\rho_q |\vec{u}_p - \vec{u}_z| d_p}{\mu_z} \cong 0 \quad (37)$$

$$F_{lift,z} = -\frac{1}{2} \rho_z \varphi_z (\vec{u}_p - \vec{u}_z) \times (\nabla \times \vec{u}_z) \cong 0 \quad (38)$$

Considering Eq. (37), the first two terms on the right side of Eq. (34) should be ignored.

Conservation of energy:

$$\nabla \cdot (\varphi_z \rho_z \vec{u}_z h_z) = -\nabla \cdot (k_z \nabla T_z) - \tau_q : \nabla \vec{u}_z + \sum_{p=1}^n \vec{Q}_{pz} \quad (39)$$

Where  $\vec{Q}_{pz} = h (\vec{u}_p - \vec{u}_z)$  is the heat exchange coefficient and  $h = \frac{6k_q \varphi_q \varphi_p N u_p}{d_p^2}$ . Also,  $Nu_p$  is calculated from Eq. (21).

Kalteh et al. [59] investigated the laminar-forced convection heat transfer of Cu-water nanofluid inside a microchannel. The Eulerian model utilized for flow simulation and governing equations was solved by FVM. The results demonstrated that the nanoparticles are distributed uniformly inside the solution domain. The two-phase model also presented a higher heat transfer augmentation compared to the single-phase model.

Laminar- and turbulent-forced convection of nanofluids inside small tubes were investigated by Chen et al. [60]. The multiphase flow was simulated using both mixture and Eulerian models and the results were compared with experimental data as well as the correlations from the literature. The obtained results for two models were quite similar, although mixture approach results showed better agreement with experimental results.



Thermal behavior and nanofluid flow at the entrance region of a pipe under constant heat flux were modeled by Göktepe et al. [61]. The results demonstrated that two-phase models predict heat transfer coefficient and friction factor with a higher accuracy at the entrance region, compared to the single-phase model. The authors also suggested that more suitable relations for nanoparticles are required to enhance the forecast accuracy of the Eulerian model.

Recently, Sadeghi et al. [62] studied nanoparticle aggregation effect on laminar convection heat transfer of alumina-water nanofluid in a circular tube. The Eulerian model was implemented according to nanoclusters Brownian motion and their fractal structure. The governing equations were solved using ANSYS CFX commercial software. The results revealed that nanoparticles size and concentration as well as fractional structure have undeniable effects on heat transfer phenomenon of nanofluid. Also, it was noted that Brownian motion can affect the convective heat transfer of nanofluids significantly.

All in all, it can be concluded that the main advantage of the Eulerian model in comparison to single-phase model is that there is no need to apply effective property models for the nanofluids [59]. However, it may not be as precise as the mixture model [17, 60].

## 2.3. Other approaches

### 2.3.1. Lattice-Boltzmann Method

Lately, Lattice-Boltzmann method or Thermal Lattice-Boltzmann method has become an attractive alternative to simulate the nanofluids flow. The gap between microscopic and macroscopic phenomena is removed by employing Lattice-Boltzmann method since it considers molecular dynamics [50]. In Lattice-Boltzmann method, the conservation equations are resolved by the assumption that the nanoparticles are microscopically located in a chain of lattices where their distributions are determined based on Boltzmann method. In the paper of Succi [63], microscopic interaction between the nanoparticles was numerically modeled utilizing a collision model and microscopic and macroscopic quantities of components were joined together. Also in [64, 65], two more different methods were employed, namely D2Q9 (two-dimensional and 9-velocity) square and D3Q19 (three-dimensional and 19-velocity) cube lattice structures. In Lattice-Boltzmann method, it is easy to deal with the complex boundaries; also, the other advantages of this method include physical representation of microscopic interactions and the existence of uniform algorithms to solve the multiphase flows [65].

For the first time, Xuan and Yao [66] proposed LBM for simulating flow and energy transport of the nanofluids. After this study, the use of this method was rapidly increased. Considering interaction forces such as Brownian, gravity-buoyancy, drag, and interaction potential forces between two phases, Qi et al. [67] studied the free convection of nanofluid using a two-phase Lattice-Boltzmann model. It was found that while Brownian, gravity-buoyancy, and interaction potential forces have positive impacts on the augmentation of free convection, drag force has a negative impact.

Karimipour et al. [68] studied laminar-forced convective heat transfer of copper-water nanofluid inside a microchannel using double-population LBM-BGK method. The obtained

results of this study were in a fair agreement with previous studies, which shows that LBM could be utilized to simulate forced convection for the nanofluids flow inside micro-sized configurations.

Recently, by employing a 2-D double multiple-relaxation-time (MRT) thermal Lattice-Boltzmann model, Zhang and Che [69] simulated the magneto-hydrodynamic (MHD) flow and heat transfer of copper water in an inclined cavity with four heat sources. The governing equations were solved using D2Q9- and D2Q5-MRT models, which was validated by previous investigations. The results showed that the inclination angle has a considerable effect on flow fields, the temperature patterns, and the local Nusselt number distributions. Moreover, it was concluded that MRT Lattice-Boltzmann method is competent for solving heat transfer of nanofluids in enclosures affected by a magnetic field.

In the end, LBM has been widely used for natural, forced, and mixed convection of nanofluids, which can be found in details [70, 71]. The results of this model have higher accuracy than the results of conventional CFD approaches. However, it seems that more research may be needed in order to find out to what extent LBM is applicable in the simulation of nanofluids flow and characteristics.

### 2.3.2. Non-homogeneous two-component model (Buongiorno model)

Buongiorno [72] investigated the effects of seven different slip mechanisms between the base fluid and nanoparticles: gravity, thermophoresis, Brownian diffusion, inertia, Magnus effect, fluid drainage and diffusiophoresis, in the absence of turbulent effects. It was demonstrated that thermophoresis and Brownian diffusion are the most influential mechanisms on nanofluids flow and heat transfer, which can affect nanoparticle concentration variations. Under such conditions, the four coupled governing equations were proposed as follows [73, 74]:

Conservation of mass:

$$\nabla \cdot (\rho_{nf} \vec{u}) = 0 \quad (40)$$

Conservation of momentum:

$$\nabla \cdot (\rho_{nf} \vec{u} \vec{u}) = -\nabla P + \nabla \cdot (\mu_{nf} \nabla \vec{u}) \quad (41)$$

Conservation of energy:

$$\nabla \cdot ((\rho c_p)_{nf} \vec{u} T) = \nabla \cdot (k_{nf} \nabla T) - c_{p_{nf}} \vec{J}_{np} \cdot \nabla T \quad (42)$$

Conservation of nanoparticles:

$$\vec{u} \cdot \nabla \phi = -\frac{1}{\rho_{np}} \nabla \cdot \vec{J}_{np} \quad (43)$$

where  $\vec{J}_{np}$  is nanoparticles flux and is defined as

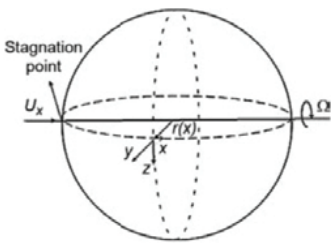
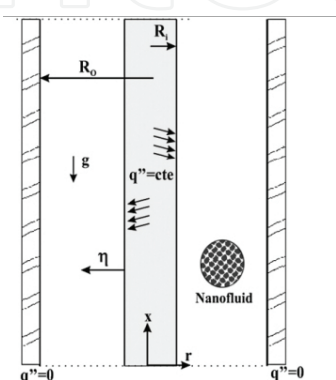
$$\vec{J}_{np} = \vec{J}_{np_{Br}} + \vec{J}_{np_T} \quad (44)$$

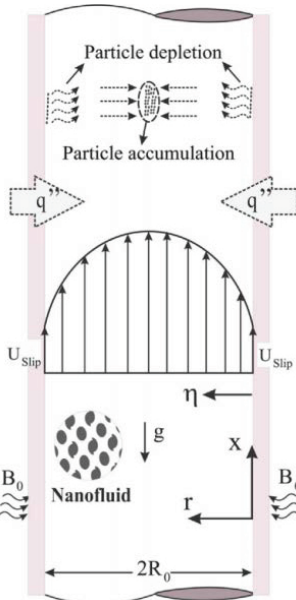
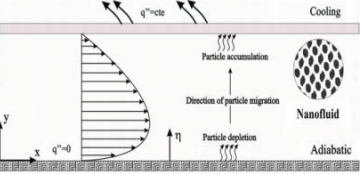
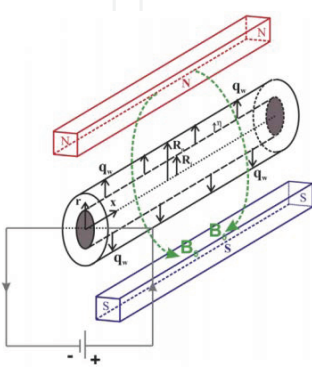
The aforementioned terms can be calculated as follows [75]:

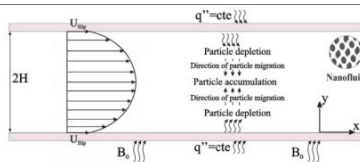
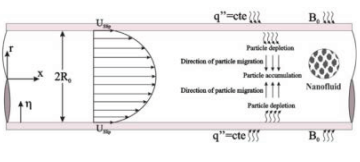
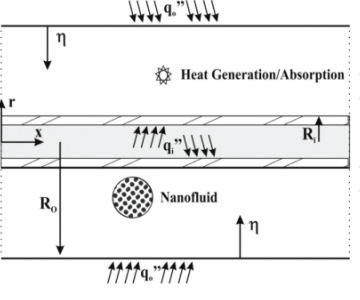
$$\vec{J}_{np_{Br}} = \frac{k_{Br} T}{3\pi\mu_f d_{np}} \quad (45)$$

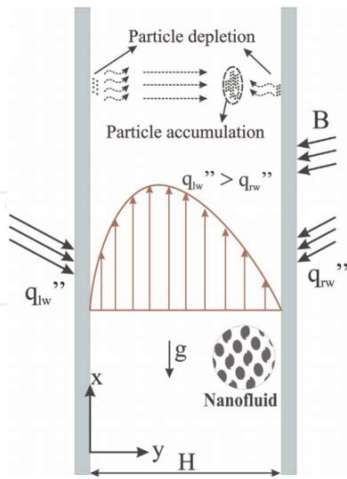
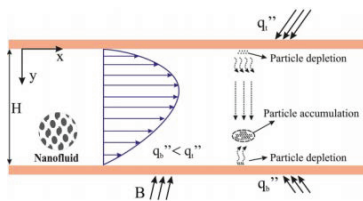
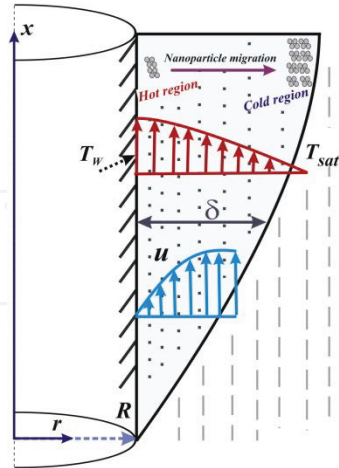
$$\vec{J}_{np_T} = 0.26 \left( \frac{k_f}{2k_f + k_{np}} \frac{\mu_f}{\rho_f} \phi \right) \quad (46)$$

where  $D$  represents the diffusion coefficient.

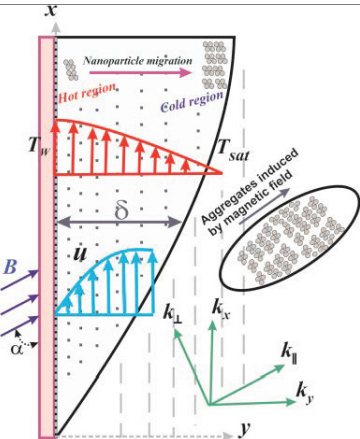
Authors	Geometry of study	Type of nanofluid	Properties	Remarks
Malvandi [79]		Non-homogeneous mixtures	$1 \text{ nm} \leq d_p \leq 100 \text{ nm}$ $0 \leq \phi \leq 0.2$	Increasing the thermophoresis is found to decrease heat transfer and concentration rates. This decrease suppresses for higher thermophoresis number. In addition, it was observed that unlike the heat transfer rate, a rise in Brownian motion leads to an increase in concentration rate
Malvandi et al. [80]		Al <sub>2</sub> O <sub>3</sub> and TiO <sub>2</sub> /water-based nanofluids	$1 \text{ nm} \leq d_p \leq 100 \text{ nm}$ $0 \leq \phi \leq 0.1$ $0.1 \leq N_{BT} \leq 10$	The buoyancy has negative effect on the efficiency of nanoparticle inclusion; however, slip velocity at the surface enhances both the heat transfer rate and the efficiency

Authors	Geometry of study	Type of nanofluid	Properties	Remarks
Malvandi, Ganji [81]		Al <sub>2</sub> O <sub>3</sub> /water nanofluid	$1\text{ nm} \leq d_p \leq 100\text{ nm}$ $0 \leq \phi \leq 0.1$ $0.1 \leq N_{BT} \leq 10$ $0 \leq Ha \leq 10$	The heat transfer rate is enhanced by the presence of the magnetic field especially for the smaller nanoparticles. Moreover, as the magnetic field strength (Ha) intensifies, the peak of the velocity profile near the walls is increased; however, the peak of the velocity profile at the core region is decreased.
Malvandi, Ganji [82]		Al <sub>2</sub> O <sub>3</sub> /water nanofluid	$1\text{ nm} \leq d_p \leq 100\text{ nm}$ $0 \leq \phi \leq 0.1$ $4 \leq N_{BT} \leq 10$	The concentration of nanoparticles is higher near the cold wall (nanoparticles accumulation), while it is lower near the adiabatic wall (nanoparticles depletion). Also, there is an optimum value for the bulk mean of nanoparticle volume fraction in which the heat transfer rate is maximum. This optimum value decreases for smaller nanoparticles.
Malvandi et al. [83]		Al <sub>2</sub> O <sub>3</sub> /water nanofluid	$1\text{ nm} \leq d_p \leq 100\text{ nm}$ $0 \leq \phi \leq 0.1$ $0.1 \leq N_{BT} \leq 10$ $0 \leq Ha \leq 15$	In the presence of the magnetic field, the velocity gradients near the wall grow, which increases the slip velocity at boundaries and thus the heat transfer rate intensifies. What is more? Increasing Ha (intensifying the magnetic field) leads to an increase in the Lorentz force (a retarding force to the transport phenomena), which tends to resist the fluid flow and thus reduces the flow's velocity.

Authors	Geometry of study	Type of nanofluid	Properties	Remarks
Malvandi, Ganji [84]		Al <sub>2</sub> O <sub>3</sub> /water nanofluid	$1\text{ nm} \leq d_p \leq 100\text{ nm}$ $0 \leq \phi \leq 0.1$ $0.2 \leq N_{BT} \leq 10$ $0 \leq Ha \leq 10$	<p>Obtained results indicated that nanoparticles move from the heated walls (nanoparticles depletion) toward the core region of the channel (nanoparticles accumulation) and construct a non-uniform nanoparticle distribution.</p> <p>Moreover, in the presence of the magnetic field, the near-wall velocity gradients increase, enhancing the slip velocity and thus the heat transfer rate and pressure drop increase.</p>
Malvandi, Ganji [85]		Al <sub>2</sub> O <sub>3</sub> /water nanofluid	$1\text{ nm} \leq d_p \leq 100\text{ nm}$ $0 \leq \phi \leq 0.1$ $0.2 \leq N_{BT} \leq 10$ $0 \leq Ha \leq 10$	<p>Nanoparticles concentration is higher in the core region of the microchannel (nanoparticles accumulation) while taking its minimum values closer to the heated wall (nanoparticles depletion). That is to say, nanoparticles move from the heated wall toward the core region and construct a non-uniform nanoparticle distribution.</p>
Moshizi et al. [86]		Al <sub>2</sub> O <sub>3</sub> /water nanofluid	$1\text{ nm} \leq d_p \leq 100\text{ nm}$ $0 \leq \phi \leq 0.1$ $0.2 \leq N_{BT} \leq 10$	<p>In the case of heat absorption, by imposing heatflux at both walls, the dimensional temperature profile becomes to be more uniform. The variations on the heat transfer coefficient enhancement in the case of heat absorption are smaller than in the case of heat generation, for a moderate range of NBT.</p> <p>Furthermore, the heat absorption boosts the pressure drops of nanofluid.</p>

Authors	Geometry of study	Type of nanofluid	Properties	Remarks
Malvandi, Ganji [87]		Al <sub>2</sub> O <sub>3</sub> /water nanofluid	$1\text{ nm} \leq d_p \leq 100\text{ nm}$ $0 \leq \phi \leq 0.1$ $0.2 \leq N_{BT} \leq 10$ $0 \leq Ha \leq 10$	It is shown that nanoparticles eject themselves from the heated walls, construct a depleted region, and accumulate in the core region, but they are more likely to accumulate toward the wall with the lower heat flux.
Malvandi et al. [88]		Al <sub>2</sub> O <sub>3</sub> /water nanofluid	$1\text{ nm} \leq d_p \leq 100\text{ nm}$ $0 \leq \phi \leq 0.1$ $0.2 \leq N_{BT} \leq 10$ $0 \leq Ha \leq 10$	The non-uniform nanoparticle distribution makes the velocities move toward the wall with the higher heat flux and enhances the heat transfer rate there. In addition, it is shown that the advantage of nanoparticle inclusion is increased in the presence of a magnetic field, though heat transfer enhancement is decreased.
Malvandi et al. [89]		Al <sub>2</sub> O <sub>3</sub> and TiO <sub>2</sub> /water-based nanofluids	$1\text{ nm} \leq d_p \leq 100\text{ nm}$ $0 \leq \phi \leq 0.06$ $0.2 \leq N_{BT} \leq 10$	The heat transfer enhancement of titania-water nanofluids is completely insignificant relative to such enhancement for alumina-water nanofluid. Therefore, alumina-water nanofluid exhibits a better performance compared to titania-water nanofluids.



Authors	Geometry of study	Type of nanofluid	Properties	Remarks
Malvandi [90]		Fe <sub>3</sub> O <sub>4</sub> -water nanofluid	$1\text{ nm} \leq d_p \leq 100\text{ nm}$ $0 \leq \phi \leq 0.06$ $0.2 \leq N_{BT} \leq 10$ $0 \leq Ha \leq 5$ $45^\circ < \alpha < 90^\circ$	A closed-form expression for the distribution of nanoparticle volume fraction has been obtained. It has been shown that the heat transfer rate is improved further when an external magnetic field exerts in the direction of the temperature gradient.

**Table 1.** Some recent studies on modified Buongiorno model.

Sheikhzadeh et al. [76] studied the effects of Brownian motion, thermophoresis, and Dufour (transport model) on laminar-free convection heat transfer of alumina-water nanofluid flow in a square enclosure. Variable thermophysical properties utilized for fluid characterization and the governing equations were discretized using FVM. The results illustrated that the Dufour effect on heat transfer is not significant. In addition, a comparison between experimental data and numerical results revealed that the transport model is in better agreement with experimental results, compared to single-phase model.

Using the same method, Bahiraei et al. [77] studied the laminar convection heat transfer of alumina-water nanofluid inside a circular tube, considering particle migration effects. The results showed that with the Reynolds number or volume fraction augmentation, the average heat transfer coefficient enhances. In addition, it was reported that by considering the particle migration effect, higher heat transfer coefficient would be achieved.

Using modified Buongiorno model, Malvandi et al. [78] investigated MHD mixed convection heat transfer for Al<sub>2</sub>O<sub>3</sub>-water nanofluid inside a vertical annular pipe. The governing equations reduced to two-point O.D.E.s, which were solved by means of the Runge-Kutta-Fehlberg scheme. The obtained results indicated that the excellence of using nanofluids for heat transfer enhancement purpose is diminished by the presence of a magnetic field. Moreover, it was noted that the imposed thermal asymmetry may change the direction of nanoparticle migration, and, hence, alters the velocity, temperature, and nanoparticle concentration profiles.

**Table 1** shows some new works on modified Buongiorno model.

### 2.3.3. Other approaches

In some other studies, novel numerical approaches have been employed to solve the governing equations of nanofluids. SPH method has been used by Mansour and Bakier [91] to study free convection within an enclosed cavity filled with Al<sub>2</sub>O<sub>3</sub> nanoparticles. The left and right walls



of the cavity had a complex-wavy geometry while upper and lower walls were both flat and insulated. Complex-wavy walls were modeled as the superposition of two sinusoidal functions. The results revealed that heat transfer performance may be optimized by tuning the wavy-surface geometry parameter in accordance with the Rayleigh number. Using optimal homotopy analysis method (OHAM), Nadeem et al. [92] examined 2-D stagnation point flow of a non-Newtonian Casson nanofluid over a convective-stretching surface. The governing non-linear partial differential equations were converted into non-linear ordinary differential equations and solved analytically using OHAM. The results showed that heat transfer rate is an increasing function of the stretching parameter, Prandtl and Biot numbers and it decreases with an increase in non-Newtonian parameter, Brownian motion, and thermophoresis.

The laminar axisymmetric flow of a nanofluid over a non-linearly stretching sheet was studied by Mustafa et al. [93], both numerically and analytically. The simultaneous effects of Brownian motion and thermophoretic diffusion of nanoparticles were taken into account. The numerical solution was computed by employing implicit finite difference scheme known as Keller-Box method. The results obtained from both solutions were in excellent agreement with each other. The results demonstrated that the effect of Brownian motion on fluid temperature and wall heat transfer rate is insignificant. Moreover, it was reported that increases in Schmidt number lead to a thinner nanoparticle volume fraction boundary layer.

### 3. Conclusion

A comprehensive review of popular methods in the simulation of the nanofluids was carried out. Different CFD approaches including single-phase, multiphase, and other methods were reviewed. For each model, the governing equations and recent literature were studied.

Conventional single-phase model was the most common method to study the convective heat transfer of nanofluids. This can be due to the fact that this model simplifies the simulation and in comparison to other models has the lowest computational cost. However, the results obtained from this model may have some deviation from the experimental data. For instance, it was reported in many studies that homogeneous model underestimates the heat transfer coefficient and Nusselt number, when compared to the dispersion and two-phase models. However, it was also revealed that using the temperature-dependent thermophysical properties in homogeneous model can lead to more realistic results. On the other hand, dispersion model for both constant and temperature-dependent properties showed promising results, compared with experimental data. This model requires less computational time compared to two-phase model. In addition, the model takes into account thermal dispersion effect, which leads to more reliable results in comparison with the homogeneous model.

Nanofluids are inherently multiphase fluids; therefore, employing two-phase model taking into account the slip velocity, Brownian motion, thermophoresis, and so forth, can lead to more appropriate results. Most of the publications confirmed that different two-phase models predict more accurate results than the homogeneous model. Also, higher values of the heat transfer coefficient were reported for two-phase models, compared to conventional single-

phase model. A vast number of studies utilized the mixture and Eulerian models, and to smaller extent VOF and Lagrangian-Eulerian models. Some publications noted that among all two-phase models, mixture model predicts more precise results compared with experimental data. However, this model has some limitation and cannot be applied in some cases. On the other hand, since VOF and Lagrangian-Eulerian models are employed less than other two-phase models, it seems that further research might be needed to assess their precision in nanofluids simulation.

In the end, LBM and non-homogeneous two-component models are rather novel approaches, used in several cases. The results predicted by these approaches showed a promising accordance with the results obtained from previous studies. Moreover, according to literature, these methods may present some well-known advantages in the modeling of nanofluids. Obviously, more attempts should be made to find the flow characteristics of nanofluids in various systems and in the presence of different modes of heat transfer in order to examine the aforementioned approaches.

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## Nomenclature

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$d$	Diameter (m)
$C_D$	Drag coefficient
$V$	volume (m <sup>3</sup> )
$F$	Force (kg m/s <sup>2</sup> )
$m$	mass (kg)
$u, v$	Flow velocity in x-y direction (m/s)
$P$	Fluid pressure (Pa)
$\vec{g}$	Gravity acceleration (m/s <sup>2</sup> )
$C_p$	Heat capacity (J/kg K)
$Nu$	Nusselt number
$Re$	Reynolds number
$h$	Sensible enthalpy (J/Kg)
$T$	Temperature (K)

$k$	Thermal conductivity (W/m K)
$t$	Time (s)
$u$	Velocity components in $x, y$ directions (m/s)

**Greek symbols**

$\alpha$	thermal diffusivity (m <sup>2</sup> /s)
$\rho$	Density (kg/m <sup>3</sup> )
$\mu$	Dynamic viscosity (Pa s)
$\phi$	Nanoparticle volume fraction
$\beta$	Thermal expansion coefficient (1/K)

**Super- and Subscripts**

Br	Brownian motion
eff	Effective
f	Fluid
Z, q	Indices
np	nanoparticle
m	Mixture
nf	Nanofluid
p	Particle
T	Thermophoresis

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