

# Simulation of natural convection and entropy generation of MHD non-Newtonian nanofluid in a cavity using Buongiorno's mathematical model

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## Abstract

In this paper, natural convection and entropy generation of non-Newtonian nanofluid, using the Buongiorno's mathematical model in a cavity in the presence of a uniform magnetic field has been analyzed by Finite Difference Lattice Boltzmann method (FDLBM). The cavity is filled with nanofluid which the mixture shows shear-thinning behavior. This study has been performed for the certain pertinent parameters of Rayleigh number ( $Ra = 10^4$  and  $10^5$ ), Hartmann number ( $Ha = 0, 15, 30$ ), buoyancy ratio number ( $N_r = 0.1, 1, \text{ and } 4$ ), power-law index ( $n = 0.4 - 1$ ), Lewis number ( $Le = 1, 5, \text{ and } 10$ ), Thermophoresis parameter ( $N_t = 0.1, 0.5, 1$ ), and Brownian motion parameter ( $N_b = 0.1, 1, 5$ ). The Prandtl number is fixed at  $Pr=1$ . The Results indicate that the augmentation of Hartmann number causes heat and mass transfer to drop. The increase in Rayleigh number enhances heat and mass transfer for various power-law indexes. The alteration of the power-law index changes heat and mass transfer. In addition, the rise of Hartmann number declines the shear-thinning behavior. The increase in the Lewis number augments mass transfer while it causes heat transfer to drop. The rise of the Thermophoresis and Brownian motion parameters ameliorate mass transfer and declines heat transfer significantly. The augmentation of buoyancy ratio number enhances heat and mass transfer. The augmentation of the power-law index declines various entropy generations in different Rayleigh numbers and Hartmann numbers. The increase in Hartmann number declines total entropy generation in different Rayleigh numbers. In addition, the rise of Rayleigh number and Hartmann number causes Bejan number to drop in various power-law indexes. The enhancement of the Lewis number provokes the total irreversibility to rise. Further, the total entropy generation increases as the buoyancy ratio number augments. It was shown that the increase in the Brownian motion and Thermophoresis parameters enhance the total irreversibility.

## 1 Introduction

### 1.1 Fuel cells (effects of nanofluid and a magnetic field)

The high request for new energy sources instead of fossil fuels has attracted many industries to fuel cell (FC) technology [1]. A Hydrogen Fuel Cell (FC) is an electro-chemical device that converts the chemical energy of hydrogen or a hydrogen rich fuel into electricity through a chemical reaction with oxygen or another oxidizing agent. Among different fuel cells, Hydrogen fuel cells, especially proton exchange membrane fuel cells (PEMFCs), have been proven to be promising energy conversion systems for automotive applications because of high power density, rapid start up, low operating temperature, high electrical energy conversion efficiency, compact size, low weight, long useful life, and the capacity to work under stop-start driving conditions [2]. The thermal management of a PEMFC is one of the most important parts. In large PEMFCs (10kW fuel cells and larger), liquid cooling, e.g. water, waterethylene-glycolor, engine oil is usually essential and in this kind of models, convection process plays the key role in heat transfer and cooling of the system [3-5]. Nanofluids have been utilized widely for improving the cooling of PEMFCs [6]. Fluids with nanoparticles suspended in them are called nanofluids where have anomalous high thermal conductivity at very low nanoparticles concentration. In addition, it was observed that the magnetic gradient force accelerates the transport process of oxygen molecules. In fact, a magnetic field influences the diffusion process of the oxygen molecules rather than the catalysis [7]. Therefore, to study the effects of these parameters (Nanofluid and a fixed magnetic field) on convection process, a benchmark study (Natural convection in a cavity) is selected in the presence of the parameters in this paper.

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### 1.2 *Natural convection in a cavity*

Flow in an enclosure driven by buoyancy force is a fundamental problem in fluid mechanics and heat transfer. This type of flow is encountered in a variety of thermal engineering applications including cooling of electronic devices and MEMS applications, furnaces, lubrication technologies, high-performance building insulation, multi-shield structures used for nuclear reactors, food processing, glass production, solar power collectors, drying technologies, fuel cells, chemical processing equipment and others. Therefore, numerous investigations have been conducted in the past on natural convection in a cavity. For instance, de Vahl Davis [8] adopted the stream function-vorticity formulation and obtained some benchmark solutions using a second-order finite difference scheme as well as the Richardson extrapolation. The results in the Rayleigh number range  $Ra = 10^3 - 10^6$  were presented. Subsequently, Le Quéré and Alziary de Roquefort [9], and Le Quéré [10] produced their solutions to the same problem but with a totally different method, i.e., the semi-implicit Chebyshev spectral method on the primitive variables system. Chenoweth and Paolucci [11,12] employed an explicit predictor-corrector finite difference method on the staggered grid to examine the gas motion in a cavity, including the effect of the aspect ratio  $A$  ( $1 \leq A \leq 10^2$ ). Barakos et al [13] studied both laminar and turbulent flows in the cavity using a finite volume approach for  $Ra = 10^3 - 10^{10}$ . Zienkiewicz et al [14] developed a characteristic-based split algorithm combined with the finite element method and applied it to the square cavity flow. The non-uniform structured mesh was used in their computation. Gjesdal et al [15] performed spectral element simulations on both square and rectangular cavities. For square cavity problem, some results under  $Ra = 10^4 - 10^8$  were listed. El-Amrani and Seaid [16] used a semi-Lagrangian Galerkin-characteristic method on the natural convection problem in a square cavity and compared results with those from Eulerian-based Galerkin finite element solvers. They provided results in the range  $Ra = 10^3 - 10^8$ .

### 1.3 *Natural convection of nanofluid in enclosures*

To observe the effect of nanofluid on natural convection process in different industries [17-22] including fuel cells, over the last decade, the analysis of natural convection in enclosures filled with nanofluids has been studied extensively using different geometries, equation models, and numerical techniques and can be used in numerous applications of engineering. Kefayati et al. [23] studied effect of SiO<sub>2</sub>/water nanofluid for heat transfer improvement in tall enclosures by Lattice Boltzmann Method. They showed that the average Nusselt number increases with volume fraction for the whole range of Rayleigh numbers and aspect ratios. In addition, the effect of nanoparticles on heat

transfer augments as the enclosure aspect ratio increases. Kefayati et al. [24] scrutinized Lattice Boltzmann simulation of natural convection in an open enclosure which subjugated to water/copper nanofluid. They mentioned the most effect of nanoparticles on heat transfer enhancement is observed at the aspect ratio of  $A=2$ . Moreover, nanoparticles influence the heat transfer less at  $Ra=10^5$  among studied Rayleigh numbers. Sajjadi et al. [25] analyzed turbulent natural convection with large-eddy simulation (LES) in a square cavity, which is filled with water/copper nanofluid. It was reported the average Nusselt number enhances with the augmentation of the nanoparticles volume fractions. Bouhaleb and Abbassi [26] studied steady two-dimensional natural convection flow of CuO-water nanofluid in an enclosure heated from one side and cooled from the ceiling. The effects of Rayleigh number and aspect ratio on flow pattern and energy transport were investigated. It was found that the effect of Rayleigh number on heat transfer is less significant when the enclosure is shallow and the influence of aspect ratio is stronger when the enclosure is tall and the Rayleigh number is high. Boualit et al. [27] carried out numerical simulations in order to analyze the effect of nanoparticles addition on the laminar natural convection in a square enclosure. The hydrodynamic structure of the flow and its thermal behavior are studied for a wide range of Rayleigh numbers and nanoparticle concentrations. The results showed an enhancement of the mean Nusselt number with an increase of nanoparticle volume fraction for all examined Rayleigh numbers.

#### *1.4 Natural convection of MHD nanofluid in a cavity*

On the other hand, in some engineering problems such as the magnetic field sensors, the magnetic storage media and the cooling systems of electronic devices, enhanced heat transfer is desirable, but the magnetic field weakens the convection process. An acceptable method in new industries which can increase heat transfer considerably is addition of nanoparticles to the base fluid. The problem, the utilization of nanoparticles in the presence of a magnetic field, on natural convection in different shapes and boundary conditions has been simulated by several researchers utilizing various numerical methods recently [28-36]. In the investigations, nanofluid is simulated, employing the single phase model without studying the thermophoresis and Brownian motion parameters. However; recently, the two-phase model is applied to study natural convection of nanofluid in the absence of the magnetic field by some researchers where the nanoparticle concentration is not uniform. In fact, Brownian motion and thermophoresis parameters have been considered [37-38]. For the all of the mentioned numerical investigations, the base fluid was assumed to be Newtonian, but it has been demonstrated by many researchers that the vast majority of nanofluids exhibit non-Newtonian, mainly shear-thinning, behavior [39-41]. Therefore, it is necessary that the effect of shear-thinning

behavior of nanofluids to be considered.

### *1.5 Entropy generation*

The optimal design of the cited industries is obtained with precision calculation of entropy generation since it clarifies energy losses in a system evidently. Entropy generation on natural convection in the presence and absence of mass transfer for different fluid flows has been scrutinized widely. Ilis et al. [42] investigated entropy generation in rectangular cavities with different aspect ratios numerically. It was demonstrated that heat transfer and fluid friction irreversibility in a cavity vary considerably with the studied aspect ratios. In addition, the total entropy generation in a cavity increases with Rayleigh number, however, the rate of increase depends on the aspect ratio. El-Maghlany et al. [43] analyzed entropy generation associated with laminar natural convection in an infinite square cavity, subjected to an isotropic heat field with various intensities for different Rayleigh numbers. Mahmoudi et al. [44] studied the entropy generation and enhancement of heat transfer in natural convection flow and heat transfer using Copper (Cu)water nanofluid in the presence of a constant magnetic field in a two dimensional trapezoidal enclosure. The results show that at  $Ra = 10^4$  and  $10^5$ , the enhancement of the Nusselt number due to presence of nanoparticles increases with the Hartman number, but at higher Rayleigh number, a reduction was observed. In addition, it was mentioned that the entropy generation decreases when the nanoparticles are present, while the magnetic field generally augments the magnitude of the entropy generation. Mejri et al. [45] examined the laminar natural convection and entropy generation in a square enclosure filled with a waterAl<sub>2</sub>O<sub>3</sub> nanofluid subjected to a magnetic field. The results demonstrated that for  $Ha = 20$  the heat transfer rate and entropy generation respectively increase and decrease with the increases of volume fraction. In addition, it was mentioned that the proper choice of Rayleigh and Hartmann numbers could be able to maximize heat transfer rate simultaneously minimizing entropy generation. Sheikholeslami and Ganji [46] investigated magnetohydrodynamic free convection flow of CuO/water nanofluid in a square enclosure with a rectangular heated body numerically using Lattice Boltzmann Method (LBM) scheme. The results showed that the heat transfer rate and dimensionless entropy generation number increase with augmentation of the Rayleigh number and the nanoparticle volume fraction, but it decreases with increase in the Hartmann number.

## 1.6 Methodology and objective

Lattice Boltzmann method (LBM) has been demonstrated to be a very effective mesoscopic numerical method to model a broad variety of complex fluid flow phenomena. This is because the main equation of the LBM is hyperbolic and can be solved locally, explicitly, and efficiently on parallel computers. However, the specific relation between the relaxation time and the viscosity has caused LBM not to have the considerable success in non-Newtonian fluid especially on energy equations. In this connection, Fu et al. [47-48] proposed a new equation for the equilibrium distribution function, modifying the LB model. Here, this equilibrium distribution function is altered in different directions and nodes while the relaxation time is fixed. Independency of the method to the relaxation time in contrast with common LBM provokes the method to solve different non-Newtonian fluid energy equations successfully as the method protects the positive points of LBM simultaneously. In addition, the validation of the method and its mesh independency demonstrates that is more capable than conventional LBM. Huilgol and Kefayati [49] derived the three dimensional equations of continuum mechanics for this method and demonstrated that the theoretical development can be applied to all fluids, whether they be Newtonian, or power law fluids, or viscoelastic and viscoplastic fluids. Kefayati [50] studied natural convection of non-Newtonian nanofluid in a cavity. Results indicated that the augmentation of the power-law index causes heat transfer to drop while increase in volume fraction of nanoparticles augments it. It was mentioned that entropy generation due to fluid friction and heat transfer rises as Rayleigh number enhances. Augmentation of volume fraction enhances entropy generations due to heat transfer and fluid friction in different power-law indexes. The total entropy generation declines slightly as power-law index increases. Kefayati [51] simulated heat transfer and entropy generation on laminar natural convection of non-Newtonian nanofluids in the presence of an external horizontal magnetic field in a square cavity. Results indicated that the augmentation of the power-law index causes heat transfer to drop in the absence of the magnetic field, by contrast, the heat transfer increases with the rise of power-law index in the presence of the magnetic field. The addition of nanoparticle augments heat transfer for multifarious studied parameters. The heat transfer dropped with the increase in Hartmann number generally and also affects the power-law index and nanoparticles influences on heat transfer. Augmentation of the volume fraction and Rayleigh number enhance all kinds of entropy generations of heat transfer, fluid friction, and the magnetic field in different studied parameters. The increase in the Hartmann number caused the total entropy generation to drop and affected the influences of the power-law index and the volume fraction on the entropy generations.

The main aim of this study is to simulate natural convection of nanofluid in

a cavity in the presence of a magnetic field as the two-phase model and shear thinning behavior have been considered simultaneously. The innovation of this paper is studying MHD non-Newtonian fluid, considering Brownian motion and thermophoresis parameters for the first time. An innovative method based on LBM has been employed to study the problem numerically. Moreover, it is endeavored to express the effects of different parameters on the flow, thermal and solutal fields. The obtained results are validated with previous numerical investigations and the effects of the main parameters (Rayleigh number, power-law index, Hartmann number, Lewis number, buoyancy ratio number, Thermophoresis parameter, and Brownian motion) on the fluid flow, heat and mass transfer, as well as entropy generations are researched.

## 2 Theoretical formulation

The geometry of the present problem is shown in Fig. 1. The temperature and concentration of the left wall have been considered to be maintained at high temperature and concentration of  $T_H$  and  $C_H$  as the right sidewall is kept at low temperature and concentration of  $T_C$  and  $C_C$ . The horizontal walls are adiabatic and impermeable. The cavity is filled with a nanofluid which shows shear-thinning behavior. A horizontal magnetic field has been applied on the flow. The Prandtl number is fixed at  $Pr=1$ . The Thermophoresis, and Brownian motion parameters also have been considered. There is no heat generation, chemical reactions, and thermal radiation. The flow is incompressible, and laminar. The density variation is approximated by the standard Boussinesq model for both temperature and concentration. The viscous dissipation and Joule heating in the energy equation are neglected. In addition, the induced magnetic field is assumed to be negligible in comparison with the external magnetic field. Moreover, the imposed and induced electrical fields are assumed to be negligible.

### 2.1 Dimensional equations

Based on the above assumptions, and applying the Boussinesq approximation, the studied equations are [50-51]:

$$\frac{\partial \bar{u}}{\partial \bar{x}} + \frac{\partial \bar{v}}{\partial \bar{y}} = 0, \quad (2.1)$$

$$\rho_f \left( \frac{\partial \bar{u}}{\partial \bar{t}} + \bar{u} \frac{\partial \bar{u}}{\partial \bar{x}} + \bar{v} \frac{\partial \bar{u}}{\partial \bar{y}} \right) = -\frac{\partial \bar{p}}{\partial \bar{x}} + \left( \frac{\partial \bar{\tau}_{xx}}{\partial \bar{x}} + \frac{\partial \bar{\tau}_{xy}}{\partial \bar{y}} \right) \quad (2.2)$$

$$\rho_f \left( \frac{\partial \bar{v}}{\partial t} + \bar{u} \frac{\partial \bar{v}}{\partial \bar{x}} + \bar{v} \frac{\partial \bar{v}}{\partial \bar{y}} \right) = - \frac{\partial \bar{p}}{\partial \bar{y}} + \left( \frac{\partial \bar{\tau}_{yy}}{\partial \bar{y}} + \frac{\partial \bar{\tau}_{xy}}{\partial \bar{x}} \right) + g_y \left[ (\rho_s - \rho_f)(\bar{C} - C_C) - \beta(1 - C_C)\rho_f(\bar{T} - T_C) \right] - \sigma B^2 \bar{v}, \quad (2.3)$$

In the above equations ( $\mathbf{u} = \bar{u}\mathbf{i} + \bar{v}\mathbf{j}$ ),  $\bar{T}$ , and  $\bar{C}$ , and  $g_y$  are the dimensional velocities, temperature, concentration, and gravity acceleration respectively.  $\beta$  is the coefficient of thermal expansion as  $\rho_f$  and  $\rho_s$  are density of fluid and solid, respectively.  $\sigma$  is electrical conductivity and  $B$  is the magnetic field. Now, let the pressure  $p$  be written as the sum  $\bar{p} = \bar{p}_s + \bar{p}_d$ , where the static part  $\bar{p}_s$  accounts for gravity alone, and  $\bar{p}_d$  is the dynamic part. Thus,

$$-\frac{\partial \bar{p}_s}{\partial y} = \rho g_y. \quad (2.4)$$

$$\begin{aligned} \frac{\partial \bar{T}}{\partial t} + \bar{u} \frac{\partial \bar{T}}{\partial \bar{x}} + \bar{v} \frac{\partial \bar{T}}{\partial \bar{y}} &= \alpha \left( \frac{\partial^2 \bar{T}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{T}}{\partial \bar{y}^2} \right) \\ &+ \delta \left\{ D_B \left( \frac{\partial \bar{C}}{\partial \bar{x}} \frac{\partial \bar{T}}{\partial \bar{x}} + \frac{\partial \bar{C}}{\partial \bar{y}} \frac{\partial \bar{T}}{\partial \bar{y}} \right) + \left( \frac{D_T}{T_C} \right) \left[ \left( \frac{\partial \bar{T}}{\partial \bar{x}} \right)^2 + \left( \frac{\partial \bar{T}}{\partial \bar{y}} \right)^2 \right] \right\} \end{aligned} \quad (2.5)$$

$D_B = \frac{k_B T_0}{3\pi d_p \mu_f}$  and  $D_T = \frac{\beta \mu_f C_0}{\rho_f}$  are the Brownian motion and the thermophoresis coefficients, respectively and  $\alpha$  is the effective thermal conductivity.  $\delta$  is a parameter defined by  $\delta = \frac{(\rho C_p)_s}{(\rho C_p)_f}$

$$\frac{\partial \bar{C}}{\partial t} + \bar{u} \frac{\partial \bar{C}}{\partial \bar{x}} + \bar{v} \frac{\partial \bar{C}}{\partial \bar{y}} = D_B \left( \frac{\partial^2 \bar{C}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{C}}{\partial \bar{y}^2} \right) + \frac{D_T}{T_C} \left( \frac{\partial^2 \bar{T}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{T}}{\partial \bar{y}^2} \right) \quad (2.6)$$

The flow domain is given by  $\Omega = (0, L) \times (0, L)$ , and the boundary  $\Gamma = \partial\Omega$ . It is the union of four disjoint subsets:

$$\Gamma_1 = \{(x, y), x = 0, 0 \leq y \leq L\}, \quad \Gamma_2 = \{(x, y), x = L, 0 \leq y \leq L\}, \quad (2.7)$$

$$\Gamma_3 = \{(x, y), 0 \leq x \leq L, y = 0\}, \quad \Gamma_4 = \{(x, y), 0 \leq x \leq L, y = L\}. \quad (2.8)$$

The boundary condition for the velocity is straightforward:

$$\mathbf{u}|_{\Gamma_1} = \mathbf{u}|_{\Gamma_2} = \mathbf{u}|_{\Gamma_3} = \mathbf{u}|_{\Gamma_4} = \mathbf{0}. \quad (2.9)$$

The boundary conditions for the temperature and concentration are:

$$T|_{\Gamma_1} = T_H, T|_{\Gamma_2} = T_C, \partial T / \partial y|_{\Gamma_3} = 0, \partial T / \partial y|_{\Gamma_4} = 0. \quad (2.10)$$



$$C|_{\Gamma_1} = C_H, C|_{\Gamma_2} = C_C, \partial C/\partial y|_{\Gamma_3} = 0, \partial C/\partial y|_{\Gamma_4} = 0. \quad (2.11)$$

In the case of the non-Newtonian power-law fluid for an incompressible flow, the general stress is given by [50-51]

$$\bar{\tau} = \bar{\eta}(II(\mathbf{A}_1))\mathbf{A}_1, \quad (2.12)$$

where  $II(\mathbf{A}_1)$  is the second invariant of the first Rivlin-Ericksen tensor  $\mathbf{A}_1$  and they are calculated as [50-51]

$$\mathbf{A}_1(\mathbf{u}) = \nabla \mathbf{u} + \nabla \mathbf{u}^T \quad (2.13)$$

$$II(\mathbf{A}_1) = \left\{ 2 \left[ \left( \frac{\partial \bar{u}}{\partial \bar{x}} \right)^2 + \left( \frac{\partial \bar{v}}{\partial \bar{y}} \right)^2 \right] + \left( \frac{\partial \bar{v}}{\partial \bar{x}} + \frac{\partial \bar{u}}{\partial \bar{y}} \right)^2 \right\}^{\frac{1}{2}}. \quad (2.14)$$

As a result, the dimensional apparent viscosity in the power-law model is as follows:

$$\bar{\eta}(II(\mathbf{A}_1)) = \left\{ 2 \left[ \left( \frac{\partial \bar{u}}{\partial \bar{x}} \right)^2 + \left( \frac{\partial \bar{v}}{\partial \bar{y}} \right)^2 \right] + \left( \frac{\partial \bar{v}}{\partial \bar{x}} + \frac{\partial \bar{u}}{\partial \bar{y}} \right)^2 \right\}^{\frac{n-1}{2}}. \quad (2.15)$$

## 2.2 Non-dimensional equations

In order to proceed to the numerical solution of the system, the following non dimensional variables are introduced.

$$t = \frac{\bar{t}}{\left(\frac{L^2}{\alpha}\right) Ra^{-0.5}}, \quad \bar{x} = x/L, \quad \bar{y} = y/L, \quad u = \frac{\bar{u}}{\left(\frac{\alpha}{L}\right) Ra^{0.5}} \quad (2.16)$$

$$v = \frac{\bar{v}}{\left(\frac{\alpha}{L}\right) Ra^{0.5}}, \quad P_d = \frac{\bar{P}_d}{\rho \left(\frac{\alpha}{L}\right)^2 Ra}, \quad \bar{T} = (T - T_C)/(T_H - T_C) \quad (2.17)$$

$$\bar{C} = (C - C_C)/(C_H - C_C) \quad (2.18)$$

By substitution of Eqs. (2.16) - (2.18) into Eqs. (2.1) - (2.6), the following system of non-dimensional equations is derived:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \quad (2.19)$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{\partial p_d}{\partial x} + \frac{Pr}{\sqrt{Ra}} \left( \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} \right), \quad (2.20)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{\partial p_d}{\partial y} + \frac{Pr}{\sqrt{Ra}} \left( \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} \right) + Pr (T - N_r C) - \frac{Pr Ha^2}{\sqrt{Ra}} v, \quad (2.21)$$

$$\begin{aligned} \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \\ \frac{1}{\sqrt{Ra}} \left[ \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + N_b \left[ \left( \frac{\partial T}{\partial x} \right) \left( \frac{\partial C}{\partial x} \right) + \left( \frac{\partial T}{\partial y} \right) \left( \frac{\partial C}{\partial y} \right) \right] + N_t \left[ \left( \frac{\partial T}{\partial x} \right)^2 + \left( \frac{\partial T}{\partial y} \right)^2 \right] \right] \end{aligned} \quad (2.22)$$

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = \frac{1}{Le\sqrt{Ra}} \left[ \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) + \frac{N_t}{N_b} \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) \right] \quad (2.23)$$

In the case of the non-Newtonian power-law fluid, the non-dimensional apparent viscosity and stresses are given by

$$\eta(II(\mathbf{A}_1)) = \left\{ 2 \left[ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \right] + \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 \right\}^{\frac{n-1}{2}}. \quad (2.24)$$

$$\begin{aligned} \tau_{xx} &= 2\eta(II(\mathbf{A}_1)) \left( \frac{\partial u}{\partial x} \right) \\ \tau_{yy} &= 2\eta(II(\mathbf{A}_1)) \left( \frac{\partial v}{\partial y} \right) \\ \tau_{xy} &= \eta(II(\mathbf{A}_1)) \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right). \end{aligned} \quad (2.25)$$

The non-dimensional parameters for the problem are as follows [50-51]:

Rayleigh number:

$$Ra = \frac{(1 - C_C)\rho_f \beta g L^3 \Delta T}{\bar{\eta} \alpha}, \quad (2.26)$$

Prandtl number:

$$Pr = \frac{\bar{\eta}}{\rho_f \alpha}, \quad (2.27)$$

Hartmann number:

$$Ha = LB \sqrt{\frac{\sigma}{\bar{\eta}}}, \quad (2.28)$$

Buoyancy ratio number:

$$N_r = \frac{(\rho_s - \rho_f) \Delta C}{\beta \Delta T \rho_f (1 - C_C)}, \quad (2.29)$$

Lewis number:

$$Le = \frac{\alpha}{D_B}, \quad (2.30)$$

Brownian motion parameter:

$$N_b = \frac{\delta D_B \Delta C}{\alpha}, \quad (2.31)$$

Thermophoresis parameter:

$$N_t = \frac{\delta D_T \Delta T}{\alpha T_C}. \quad (2.32)$$

### 3 Entropy generation

#### 3.1 Dimensional equations

In the studied problem, the irreversibility is generated through heat transfer, fluid friction and mass transfer. As a result, the total entropy is the sum of the irreversibilities due to thermal gradients, viscous dissipation and concentration gradients as follows [52-55]:

$$\bar{S}_S = \bar{S}_F + \bar{S}_T + \bar{S}_D + \bar{S}_G. \quad (3.1)$$

Where the entropy generations due to fluid friction ( $\bar{S}_F$ ), heat transfer ( $\bar{S}_T$ ), magnetic field ( $\bar{S}_G$ ), and mass transfer ( $\bar{S}_D$ ) is calculated as follows:

$$\bar{S}_F = \frac{\bar{\eta}}{T_0} \left[ 2 \left( \frac{\partial \bar{u}}{\partial \bar{x}} \right)^2 + 2 \left( \frac{\partial \bar{v}}{\partial \bar{y}} \right)^2 + \left( \frac{\partial \bar{u}}{\partial \bar{y}} + \frac{\partial \bar{v}}{\partial \bar{x}} \right)^2 \right] . \quad (3.2)$$

$$\bar{S}_T = \frac{k}{T_0^2} \left[ \left( \frac{\partial \bar{T}}{\partial \bar{x}} \right)^2 + \left( \frac{\partial \bar{T}}{\partial \bar{y}} \right)^2 \right] . \quad (3.3)$$

$$\bar{S}_G = -\frac{\sigma B^2}{T_0} \bar{v}^2, \quad (3.4)$$

$$\bar{S}_D = \frac{RD_B}{C_0} \left[ \left( \frac{\partial \bar{C}}{\partial \bar{x}} \right)^2 + \left( \frac{\partial \bar{C}}{\partial \bar{y}} \right)^2 \right] + \frac{RD_B}{T_0} \left[ \left( \frac{\partial \bar{C}}{\partial \bar{x}} \right) \left( \frac{\partial \bar{T}}{\partial \bar{x}} \right) + \left( \frac{\partial \bar{C}}{\partial \bar{y}} \right) \left( \frac{\partial \bar{T}}{\partial \bar{y}} \right) \right] , \quad (3.5)$$

$k$  is the thermal conductivity and  $R$  is the Gas constant.  $T_0$  and  $C_0$  are bulk temperature and bulk concentration respectively and could be calculated as

$$T_0 = \frac{T_H + T_C}{2}, \quad C_0 = \frac{C_H + C_C}{2}, \quad (3.6)$$

An important measure of the entropy field is Bejan number (Be) which is defined as the ratio between entropy generations due to heat and mass transfer irreversibilities to the total entropy generation as follow

$$\overline{Be} = \frac{\bar{S}_T + \bar{S}_D}{\bar{S}_S} . \quad (3.7)$$

### 3.2 Non-dimensional equations

The local dimensionless entropy generations with consideration to non-dimensional variables of Eqs. (2.16) - (2.18) can be acquired as follows:

$$S_S = S_F + S_T + S_D + S_G \quad (3.8)$$

$$S_F = \Phi_I \left[ 2 \left( \frac{\partial u}{\partial x} \right)^2 + 2 \left( \frac{\partial v}{\partial y} \right)^2 + \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 \right] , \quad (3.9)$$

$$S_T = \left[ \left( \frac{\partial T}{\partial x} \right)^2 + \left( \frac{\partial T}{\partial y} \right)^2 \right] , \quad (3.10)$$

$$S_D = \Phi_{II} \left[ \left( \frac{\partial C}{\partial x} \right)^2 + \left( \frac{\partial C}{\partial y} \right)^2 \right] + \Phi_{III} \left[ \left( \frac{\partial C}{\partial x} \right) \left( \frac{\partial T}{\partial x} \right) + \left( \frac{\partial C}{\partial y} \right) \left( \frac{\partial T}{\partial y} \right) \right] , \quad (3.11)$$

$$S_G = \Phi_I Ha^2 v^2, \quad (3.12)$$

$$\Phi_I = \frac{\eta T_0}{k} \left( \frac{\alpha}{L\Delta T} \right)^2 Ra = \frac{\left\{ 2 \left[ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \right] + \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 \right\}^{\frac{(n-1)}{2}} T_0}{k} \left( \frac{\alpha}{L\Delta T} \right)^2 Ra, \quad (3.13)$$

$$\lambda = \frac{T_0}{k} \left( \frac{\alpha}{L\Delta T} \right)^2 \quad (3.14)$$

$$\Phi_{II} = \frac{RD_B T_0}{k C_0} \left( \frac{\Delta C}{\Delta T} \right)^2 \quad (3.15)$$

$$\Phi_{III} = \frac{RD_B}{k} \left( \frac{\Delta C}{\Delta T} \right) \quad (3.16)$$

It should be mentioned that the variables of  $\Phi_{II}$ ,  $\Phi_{III}$ ,  $\lambda$  is taken constant [52-55] and they are  $\Phi_{II} = 0.5, \Phi_{III} = 0.01, \lambda = 0.01$ . The local non-dimensional Bejan number is calculated as follows:

$$Be = \frac{S_T + S_D}{S_S}, \quad (3.17)$$

The total dimensionless entropy generations are obtained by numerical integration of the local dimensionless entropy generation over the entire cavity volume. It is given by:

$$S_{F,tot} = \int_0^1 \int_0^1 S_F dx dy, \quad S_{T,tot} = \int_0^1 \int_0^1 S_T dx dy, \quad S_{D,tot} = \int_0^1 \int_0^1 S_D dx dy, \quad (3.18)$$

$$S_{G,tot} = \int_0^1 \int_0^1 S_G dx dy, \quad S_{S,tot} = \int_0^1 \int_0^1 S_S dx dy, \quad (3.19)$$

Similarity, average Bejan number can be obtained as follow

$$Be_{avg} = \int_0^1 \int_0^1 Be dx dy. \quad (3.20)$$

#### 4 The numerical method

The FDLBM equations and their relationships with continuum equations have been explained in details in Huilgol and Kefayati [49]. Here, just a brief description about the main equations would be cited. In addition, the applied algorithm has been described and the studied problem equations in the FDLBM

are mentioned.

#### 4.1 The Continuity and Momentum equations

To have the continuity and momentum equations, a discrete particle distribution function  $f_\alpha$  is defined over a D2Q9 lattice where it should satisfy an evolution equation:

$$\frac{\partial f_\alpha}{\partial t} + \boldsymbol{\xi}_\alpha \cdot \nabla_{\mathbf{x}} f_\alpha - F_\alpha = -\frac{1}{\varepsilon \phi} (f_\alpha - f_\alpha^{eq}), \quad (4.1)$$

where  $\varepsilon$  is a small parameter to be prescribed when numerical simulations are considered.

Associated to each node is a lattice velocity vector  $\boldsymbol{\xi}_\alpha$ . It is defined as follows:

$$\boldsymbol{\xi}_\alpha = \begin{cases} (0, 0), & \alpha = 0, \\ \sigma(\cos \theta_\alpha, \sin \theta_\alpha) & \alpha = 1, 3, 5, 7, \\ \sigma\sqrt{2}(\cos \theta_\alpha, \sin \theta_\alpha), & \alpha = 2, 4, 6, 8. \end{cases} \quad (4.2)$$

Here, the angles  $\theta_\alpha$  are defined through  $\theta_\alpha = (\alpha - 1)\pi/4$ ,  $\alpha = 1, \dots, 8$ . The constant  $\sigma$  has to be chosen with care for it affects numerical stability; its choice depends on the problem. The method for finding the parameter  $\sigma$  which satisfies the Courant-Friedrichs-Lewy (CFL) condition is described in [49].

The equilibrium distribution function,  $f_\alpha^{eq}$ , is different from the conventional ones adopted by previous researchers, who normally expand the Maxwellian distribution function. In the present approach, we expand  $f_\alpha^{eq}$  as a quadratic in terms of  $\boldsymbol{\xi}_\alpha$ , using the notation of linear algebra:

$$f_\alpha^{eq} = A_\alpha + \boldsymbol{\xi}_\alpha \cdot \mathbf{B}_\alpha + (\boldsymbol{\xi}_\alpha \otimes \boldsymbol{\xi}_\alpha) : \mathbf{C}_\alpha, \quad \alpha = 0, 1, 2, \dots, 8. \quad (4.3)$$

Here, the scalars  $A_\alpha$  are defined through

$$A_0 = \rho - \frac{2p}{\sigma^2} - \frac{\rho|\mathbf{u}|^2}{\sigma^2} + \frac{\tau_{xx} + \tau_{yy}}{\sigma^2}, \quad A_\alpha = 0, \quad \alpha = 1, 2, \dots, 8. \quad (4.4)$$

The vectors  $\mathbf{B}_\alpha$  are given by

$$\mathbf{B}_1 = \frac{\rho\mathbf{u}}{2\sigma^2} = \mathbf{B}_\alpha, \quad \alpha = 1, 3, 5, 7; \quad \mathbf{B}_\alpha = \mathbf{0}, \quad \alpha = 0, 2, 4, 6, 8. \quad (4.5)$$

Next, the matrices  $\mathbf{C}_\alpha$  are such that  $\mathbf{C}_0 = 0$ ;  $\mathbf{C}_1 = \mathbf{C}_\alpha$ ,  $\alpha = 1, 3, 5, 7$ ;  $\mathbf{C}_2 = \mathbf{C}_\alpha$ ,  $\alpha = 2, 4, 6, 8$ , where

$$\mathbf{C}_1 = \begin{bmatrix} C_{11} & 0 \\ 0 & C_{22} \end{bmatrix}, \quad C_{11} = \frac{1}{2\sigma^4}(p + \rho u^2 - \tau_{xx}), \quad C_{22} = \frac{1}{2\sigma^4}(p + \rho v^2 - \tau_{yy}), \quad (4.6)$$

$$\mathbf{C}_2 = \begin{bmatrix} 0 & C_{12} \\ C_{21} & 0 \end{bmatrix}, \quad C_{12} = C_{21} = \frac{1}{8\sigma^4}(\rho uv - \tau_{xy}). \quad (4.7)$$

In order to derive the macroscopic equations for an incompressible continuous medium in the presence of a body force, it has been shown that [49-51] the functions  $F_\alpha$  in (4.1) must be such that

$$\sum_{\alpha=0}^8 F_\alpha = 0. \quad (4.8)$$

In turn, this guarantees that the conservation of mass equation is satisfied. Next, one requires that

$$\sum_{\alpha=0}^8 F_\alpha \boldsymbol{\xi}_\alpha = \rho \mathbf{b}, \quad (4.9)$$

where  $\rho \mathbf{b}$  is the body force. Thus, one choice for the set of  $F_\alpha$  is:

$$F_0 = 0, \quad F_1 = \frac{1}{2\sigma^2} \rho \mathbf{b} \cdot \boldsymbol{\xi}_1, \quad F_3 = \frac{1}{2\sigma^2} \rho \mathbf{b} \cdot \boldsymbol{\xi}_3, \quad (4.10a)$$

$$F_5 = \frac{1}{2\sigma^2} \rho \mathbf{b} \cdot \boldsymbol{\xi}_5, \quad F_7 = \frac{1}{2\sigma^2} \rho \mathbf{b} \cdot \boldsymbol{\xi}_7. \quad (4.10b)$$

$$F_\alpha = 0, \quad \alpha = 2, 4, 6, 8. \quad (4.10c)$$

One notes that  $F_1 = -F_5$ ,  $F_3 = -F_7$ .

In this problem, the non-dimensional body force is as follows:

$$\rho \mathbf{b} = \frac{\text{Pr}(T - NrC) - \frac{\text{Pr} Ha^2}{\sqrt{\text{Ra}}} v}{2\sigma^2} \mathbf{j} \quad (4.11)$$

## 4.2 The Energy Equation

In order to obtain the energy equation, an internal energy distribution function  $g_\alpha$  is introduced and it is assumed to satisfy an evolution equation similar to that for  $f_\alpha$ . Thus,

$$\frac{\partial g_\alpha}{\partial t} + \boldsymbol{\xi}_\alpha \cdot \nabla_{\mathbf{x}} g_\alpha - G_\alpha = -\frac{1}{\varepsilon\phi}(g_\alpha - g_\alpha^{eq}). \quad (4.12)$$

Here,  $g_\alpha^{eq}$  has a monomial expansion:

$$g_\alpha^{eq} = D_\alpha + \boldsymbol{\xi}_\alpha \cdot \mathbf{E}_\alpha, \quad (4.13)$$

One way of satisfying the above is to assume, as before, that the scalars are given by  $D_\alpha = D_1$ ,  $\alpha = 1, 3, 5, 7$ , and  $D_\alpha = D_2$ ,  $\alpha = 2, 4, 6, 8$ . In this problem, the non-dimensional parameters are obtained as follows:

$$D_0 = T, \quad D_1 = 0, \quad D_2 = 0. \quad (4.14)$$

Regarding the vectors, it is assumed that  $\mathbf{E}_0 = \mathbf{0}$ ,  $\mathbf{E}_\alpha = \mathbf{E}_1$ ,  $\alpha = 1, 3, 5, 7$ ;  $\mathbf{E}_\alpha = \mathbf{E}_2$ ,  $\alpha = 2, 4, 6, 8$ , where

$$\mathbf{E}_1 = \frac{\left(\mathbf{u}T - \frac{1}{\sqrt{Ra}}\left(\frac{\partial \mathbf{T}}{\partial \mathbf{x}} + N_b\left(T\frac{\partial \mathbf{C}}{\partial \mathbf{x}}\right) + N_t\left(T\frac{\partial \mathbf{T}}{\partial \mathbf{x}}\right)\right)\right)}{2\sigma^2}. \quad (4.15)$$

Finally,  $G_\alpha = 0$ .

## 4.3 The Concentration Equation

In order to obtain the concentration equation, an internal concentration distribution function  $h_\alpha$  is introduced and it is assumed to satisfy an evolution equation similar to that for  $f_\alpha$ . Thus,

$$\frac{\partial h_\alpha}{\partial t} + \boldsymbol{\xi}_\alpha \cdot \nabla_{\mathbf{x}} h_\alpha - H_\alpha = -\frac{1}{\varepsilon\phi}(h_\alpha - h_\alpha^{eq}). \quad (4.16)$$

Here,  $h_\alpha^{eq}$  has a monomial expansion:

$$h_\alpha^{eq} = M_\alpha + \boldsymbol{\xi}_\alpha \cdot \mathbf{N}_\alpha, \quad (4.17)$$

One way of satisfying the above is to assume, as before, that the scalars are given by  $M_\alpha = M_1$ ,  $\alpha = 1, 3, 5, 7$ , and  $M_\alpha = M_2$ ,  $\alpha = 2, 4, 6, 8$ . In this



problem, the non-dimensional parameters are obtained as follows:

$$M_0 = C, \quad M_1 = 0, \quad M_2 = 0. \quad (4.18)$$

Regarding the vectors, it is assumed that  $\mathbf{N}_0 = \mathbf{0}$ ,  $\mathbf{N}_\alpha = \mathbf{N}_1$ ,  $\alpha = 1, 3, 5, 7$ ;  $\mathbf{N}_\alpha = \mathbf{N}_2$ ,  $\alpha = 2, 4, 6, 8$ , where

$$\frac{\left( \mathbf{u} C - \frac{1}{Le\sqrt{Ra}} \left( \frac{\partial \mathbf{C}}{\partial \mathbf{x}} + \frac{N_i}{N_b} \frac{\partial \mathbf{T}}{\partial \mathbf{x}} \right) \right)}{2\sigma^2} \quad (4.19)$$

Finally,  $H_\alpha = 0$ .

The local and the average Nusselt numbers at the hot wall with the utilization of the dimensionless parameters are calculated as

$$Nu = \left( -\frac{\partial T}{\partial x} \right)_{x=0} \quad (4.20)$$

$$Nu_{avg} = \int_0^1 Nu dy \quad (4.21)$$

The local and the average Sherwood numbers with the utilization of the dimensionless parameters at the hot wall are calculated as

$$Sh = \left( -\frac{\partial C}{\partial x} \right)_{x=0} \quad (4.22)$$

$$Sh_{avg} = \int_0^1 Sh dy \quad (4.23)$$

Because of considering power-law index effects on different parameters exactly, normalized average Nusselt and Sherwood numbers on the hot wall are defined. The normalized average Nusselt and Sherwood numbers express Nusselt and Sherwood numbers at any power-law indexes to the Newtonian fluid ones which are written as follows:

$$Nu_{avg}^*(n) = \frac{Nu_{avg}(n)}{Nu_{avg}(n=1)} \quad (4.24)$$

$$Sh_{avg}^*(n) = \frac{Sh_{avg}(n)}{Sh_{avg}(n=1)} \quad (4.25)$$

## 5 Code validation and grid independence

Finite Difference Lattice Boltzmann Method (FDLBM) scheme is utilized to simulate entropy generation of laminar natural convection in a cavity that is filled with non-Newtonian nanofluid. The Buongiorno's mathematical model has been employed in this simulation where the Thermophoresis and Brownian motion parameters have been studied. The Prandtl number is fixed at  $Pr=1$ . This problem is investigated at different Rayleigh numbers of ( $Ra=10^4$  and  $10^5$ ), power-law index ( $n=0.4-1$ ), buoyancy ratio number ( $N_r = 0.1, 1, \text{ and } 4$ ), Hartmann numbers ( $Ha = 0, 15, 30$ ), Lewis number ( $Le = 1, 5, \text{ and } 10$ ), Thermophoresis parameter ( $N_t = 0.1, 0.5, 1$ ), and Brownian motion parameter ( $N_b=0.1, 1, 5$ ). An extensive mesh testing procedure was conducted to guarantee a grid independent solution. Seven different mesh combinations were explored for the case of  $Ra = 10^5$ ,  $Ha = 15$ ,  $n=1$ ,  $Le = 1$  and  $N_r = N_t = N_b = 0.1$ . It was confirmed that the grid size ( $150*150$ ) ensured a grid independent solution as portrayed in Table 1. To check the accuracy of the present results, the present code for Newtonian fluid is validated with published studies on the natural convection in a cavity. The results are compared in Table 2 as it shows an agreement between present and previous studies. To validate the precision of the present consequences for calculation of entropy, the obtained results are validated with the study of Ilis et al. [42] in Fig.2. FDLBM is applied for non-Newtonian natural convection and entropy generation of non-Newtonian nanofluid and MHD non-Newtonian nanofluid in the absence of mass transfer by the author recently [50-51] which demonstrates the accuracy of the utilized code for non-Newtonian nanofluid properly.

## 6 Results and discussion

### 6.1 Effects of Rayleigh number, power-law index and Hartmann number on fluid flow, heat and mass transfer

Fig.3 presents the isotherms, streamlines and the isoconcentrations for different power-law indexes and Hartmann numbers at  $Ra = 10^5$ ,  $N_r = N_t = N_b = 0.1$ , and  $Le=1$ . The isotherm of  $T=0.8$  can indicate the effect of power-law index on the isotherms properly at  $Ha=0$  as the distance of the isotherm of  $T=0.8$  from the hot wall drops with the increment of power-law index and therefore the convection process becomes weak. In addition, the streamline of  $\psi=-0.035$  diminishes gradually as power-law index enhances and demonstrates that the convection process falls at  $Ha=0$  with the enhancement of power-law index. The isoconcentration of  $C=0.9$  at  $Ha=0$ , shows the influence of power-law index clearly where it transfers shorter distance between

the cold and hot walls and therefore demonstrates the convection of the mass transfer decreases with the augmentation of the power-law index noticeably. It is evident that the increase in Hartmann number causes the gradients of isotherms and isoconcentrations on the hot wall to drop considerably. The rise of the Hartmann number provokes the movement of the isotherms and isoconcentrations between the hot and cold walls to alter. The trend demonstrates that the convection process is becoming weak with the enhancement of Hartmann number. Moreover, it shows that the enhancement of power-law index in various Hartmann number declines the gradients of the isotherms and isoconcentrations. The fixed streamlines values of  $\psi = -0.035, -0.0278$  and  $-0.0195$  demonstrate that the rise of power-law index declines the convection process for Hartmann numbers of  $Ha=0, 15,$  and  $30,$  respectively.

Fig.4 illustrates influence of power-law index and Rayleigh numbers on the distribution of velocity in the middle of the cavity while local Nusselt and Sherwood numbers on the hot wall are studied at  $N_r = N_t = N_b = 0.1,$   $Le=1,$  and  $Ha=0.$  It shows that the profile of the velocity, the local Nusselt and Sherwood numbers enhance generally as the Rayleigh number augments. It depicts that the local Nusselt number drops by the rise of the power-law index considerably. But, the local Nusselt number declines considerably from  $n=0.4$  to  $0.6$  compared to other power-law indexes. Moreover, the effect of power-law index on the local Nusselt number is not uniform on the hot wall. In another words, the effect of the power-law index on the local Nusselt number drops along the hot wall with the rise of the  $Y$  where the local Nusselt number for different power-law indexes are nearly the same at  $Y > 0.8.$  The local Sherwood number shows similar behavior of the local Nusselt number as it decreases with the enhancement of the power-law index. In addition, the effect of the power-law index on the local Sherwood number drops along the hot wall where in the second half of the hot wall the local Sherwood numbers are nearly the same for various power-law indexes. The vertical velocity in different power-law indexes displays that the maximum vertical velocity drops and the curvy shape of the distribution declines due to the increase in power-law index. However, the effect of power-law index on the vertical velocity from  $n=0.4$  to  $0.6$  is more considerable than other power-law indexes.

Fig.5 depicts the distribution of velocity in the middle of the cavity and the local Nusselt and Sherwood numbers on the hot wall are studied in different Hartmann numbers and Rayleigh numbers. It is apparent the augmentation of the Hartmann number causes the local Nusselt and Sherwood numbers to drop significantly as the decline is more sever from  $Ha=15$  to  $30.$  However, it depicts that the effect of the Hartmann number on the local Nusselt and Sherwood numbers decrease steadily from the bottom section of the hot wall to the upper part. The cited trend is clear at  $0.8 < Y < 1$  where the Nusselt and Sherwood numbers are nearly the same for different Hartmann numbers. The amplitudes of vertical velocities distributions, which are located close to the

sidewalls, diminish with the increase of Hartmann number. The phenomenon demonstrates that the convection process is weakened by the enhancement of the Hartmann number.

Fig.6 shows the average Nusselt and Sherwood numbers as well as the normalized average Nusselt and Sherwood numbers on the hot wall in different Rayleigh numbers, Hartmann numbers and power-law indexes. The average Nusselt and Sherwood numbers show that heat and mass transfer enhance with the rise of Rayleigh number generally. Furthermore, it demonstrates that heat and mass transfer decrease markedly as Hartmann number increases in various Rayleigh numbers and power-law indexes. At  $Ha=0$ , the increase in power-law index provokes heat and mass transfer to drop in different Rayleigh numbers. At  $Ha=15$ , the average Nusselt and Sherwood numbers decrease due to the augmentation of power-law index at  $Ra=10^5$ . The normalized average Nusselt and Sherwood numbers at  $Ha=15$  demonstrate that the effect of power-law index on heat and mass transfer drops and augments, respectively, compared to  $Ha=0$ . At  $Ha=30$ , it is clear that the effect of power-law index on the average Nusselt and Sherwood numbers drop considerably, compared to  $Ha=0$  and 15. In addition, the enhancement of power-law index causes the average Nusselt and Sherwood numbers to drop at  $Ra=10^5$ . Further, the average Nusselt and Sherwood number increases and drops with the rise of the power-law index at  $Ha=30$  and  $Ra=10^4$ .

## 6.2 *Effects of buoyancy ratio on fluid flow, heat and mass transfer*

Fig.7 displays the isotherms, streamlines and the isoconcentrations for different buoyancy ratios at  $Ra = 10^5$ ,  $N_t = N_b = 0.1$ ,  $Ha=0$  and  $Le=1$ . The comparison between the isotherms demonstrates the rise of the buoyancy ratio causes the gradient of the isotherms on the hot wall to increase significantly. Hence, the pattern clarifies that the augmentation of buoyancy ratio enhances heat transfer. Moreover, the trend is observed in isoconcentrations as they incline to the hot wall and their gradient augments noticeably. As a result, mass transfer similar to heat transfer is improved by the increase in buoyancy ratio. The shapes of the streamlines in different buoyancy ratios can prove the cited result in the isotherms and isoconcentrations properly since a fixed value of the streamline ( $\psi=-0.035$ ) expands with the increase in the buoyancy ratio.

Fig.8 indicates the distribution of velocity in the middle of the cavity and the local Nusselt and Sherwood numbers on the hot wall are studied for different Buoyancy ratio numbers ( $N_r$ ) at  $Ra = 10^5$ ,  $N_t = N_b = 0.1$ ,  $Ha=0$  and  $Le=1$ . It depicts that the local Nusselt and Sherwood numbers on the hot wall augment gradually as the buoyancy ratio increases. The vertical velocity displays that the maximum values of the vertical velocity at  $0 < Y < 0.2$  and  $0.8 < Y < 1$

enhance while the vertical velocities at  $0.2 < Y < 0.8$  shows equivalent values. It demonstrates that the convection process is augmented with the increase in the buoyancy ratio.

Fig.9 exhibits the average Nusselt and Sherwood numbers on the hot wall are studied for different Buoyancy ratio numbers ( $N_r$ ) at  $Ra = 10^5$ ,  $n=1$ ,  $N_t = N_b = 0.1$ ,  $Ha=0$  and  $Le=1$ . It shows that average Nusselt and Sherwood numbers increase with the rise of buoyancy ratio.

### 6.3 *Effects of Thermophoresis and Brownian motion parameters on fluid flow, heat and mass transfer*

Fig.10 demonstrates the isotherms, streamlines and the isoconcentrations for different Thermophoresis and Brownian motion parameters at  $Ra = 10^5$ ,  $N_r=0.1$ ,  $Ha=0$  and  $Le=1$ . The comparison between the isotherms demonstrates the rise of the buoyancy ratio causes the gradient of the isotherms on the hot wall to drop significantly. Hence, the pattern clarifies that the augmentation of Thermophoresis and Brownian motion parameters declines heat transfer. However, the gradient of the isoconcentrations augments noticeably with the increase in the Thermophoresis and Brownian motion parameters. As a result, mass transfer is ameliorated by the increase in buoyancy ratio. The shapes of the streamlines in different Brownian motion and Thermophoresis parameters can prove the amelioration of the convection process since a fixed value of the streamline ( $\psi=-0.035$ ) expands with the increase in the buoyancy ratio.

Fig.11 reveals influence of Brownian motion ( $N_b$ ) and Thermophoresis parameters ( $N_t$ ) on the distribution of velocity in the middle of the cavity while local Nusselt and Sherwood numbers on the hot wall are studied at  $Ra = 10^5$ ,  $N_r=0.1$ ,  $Ha=0$  and  $Le=1$ . It shows that the local Nusselt number on the hot wall drops gradually as the Brownian motion and Thermophoresis parameters increase. In contrast with the local Nusselt number, the local Sherwood number enhances considerably as the Brownian motion and Thermophoresis parameters rise. The vertical velocity indicates that the convection process improves with the increase in the Brownian motion and Thermophoresis parameters as the vertical velocity augments significantly.

Fig.12 depicts the average Nusselt and Sherwood numbers in different Brownian motion and Thermophoresis parameters on the hot wall at  $Ra = 10^5$ ,  $N_r=0.1$ ,  $Ha=0$  and  $Le=1$ . It shows that average Nusselt number decreases and Sherwood number increases with the rise of Brownian motion and Thermophoresis parameters.

#### 6.4 Effects of Lewis number on fluid flow, heat and mass transfer

Fig.13 illustrates the isotherms, streamlines and the isoconcentrations for different Lewis numbers at  $Ra = 10^5$ ,  $N_t = N_b = N_r = 0.1$ , and  $Ha=0$ . The contours exhibit that the density of the isoconcentrations on the hot wall grows with the increase in Lewis numbers for multifarious Rayleigh numbers and power-law indexes. The pattern confirms that mass transfer enhances with the rise of Lewis number generally without consideration to power-law index and Rayleigh number values. But, the gradient of the isotherms declines marginally with the augmentation of Lewis number.

Fig.14 discloses the effect of Lewis number on the distribution of velocity in the middle of the cavity while local Nusselt and Sherwood numbers on the hot wall are studied at  $Ra = 10^5$ ,  $N_t = N_b = N_r = 0.1$ , and  $Ha=0$ . The local Sherwood number confirms the trends of the isoconcentrations where it enhances with the rise of Lewis number substantially. On the other hand, the local Nusselt number decreases when the Lewis number rises. The vertical velocity shows that the convection process is not affected considerably by the increase in the Lewis number as the vertical velocity is almost the same for different Lewis numbers.

Fig.15 depicts the average Nusselt and Sherwood numbers in different Lewis numbers on the hot wall at  $Ra = 10^5$ ,  $N_t = N_b = N_r = 0.1$ , and  $Ha=0$ . It is clear that average Nusselt numbers for different power-law indexes and Rayleigh numbers decreases with the enhancement of Lewis number, but the trend is completely different for the average Sherwood number. In fact, the average Sherwood number rises noticeably as Lewis number augments.

#### 6.5 Effects of power-law index, Rayleigh number and Hartmann numbers on entropy generation

Fig.16 presents local entropy generation due to heat transfer ( $S_T$ ) for different Rayleigh numbers, power-law indexes, and Hartmann numbers at  $N_t = N_b = N_r = 0.1$ , and  $Le=1$ . The enhancement of Rayleigh number in multifarious power-law indexes and Hartmann numbers augment the local entropy generation due to heat transfer. The local entropy generation due to heat transfer in different Hartmann numbers illustrates that the increase in power-law index causes the gradient of the entropy generation and the maximum value of the entropy generation to drop while the shape of the local entropy generation follow the same pattern in the enclosure. In addition, the rise of Rayleigh number augments the entropy generations due to heat transfer considerably and the dense of the irreversibility of heat transfer increases significantly. The increase

in Hartmann number declines the value of the local entropy generation due to heat transfer in different Rayleigh numbers and power-law indexes. The rise of power-law index weakens the local entropy generation in various Hartmann numbers; although, the effect of power-law index on the local entropy generation decreases with the rise of Hartmann number.

Fig.17 illustrates local entropy generation due to fluid friction ( $S_F$ ) for different Rayleigh numbers, power-law indexes, and Hartmann numbers at  $N_t = N_b = N_r = 0.1$ , and  $Le=1$ . It demonstrates that the increase in Rayleigh number for various power-law indexes and Hartmann numbers causes the high values of the entropy generation to concentrate on the side walls and the local entropy generation to enhance generally. Moreover, it is clear that there are high values of the local entropy generation close to the horizontal walls at  $Ra = 10^4$  while the regions are completely vanished at  $Ra = 10^5$ . The maximum values of the local entropy generation due to the fluid friction can exhibit the influence of the Rayleigh number evidently. It also exhibits that the local entropy generation due to the fluid friction drops considerably as the power-law index enhances in multifarious Hartmann numbers and Rayleigh numbers. However, the irreversibility follows the same patterns and shapes for different power-law indexes. The Hartmann number affects the irreversibility due to the fluid friction significantly. It depicts that the  $S_F$  drops noticeably when the Hartmann number increases.

Fig.18 displays local entropy generation due to mass transfer ( $S_D$ ) for different Rayleigh numbers, power-law indexes, and Hartmann numbers at  $N_t = N_b = N_r = 0.1$ , and  $Le=1$ . It shows that the rise of the Rayleigh number enhances the  $S_D$  considerably in different power-law indexes and Hartmann numbers. At  $Ha=0$ , the  $S_D$  weakens as the power-law index rises in different Rayleigh numbers. The increase in Hartmann number provokes the  $S_D$  to drop. The rise of Hartmann number changes the pattern of  $S_D$  at  $Ra=10^4$  where the maximum values transfer from sidewalls to horizontal walls. In addition, the enhancement of Hartmann number declines the effect of power-law index on the  $S_D$ .

Fig.19 displays local entropy generation due to magnetic field ( $S_G$ ) for different Rayleigh numbers, power-law indexes, and Hartmann numbers at  $N_t = N_b = N_r = 0.1$ , and  $Le=1$ . It shows that the rise of Hartmann number augments the local entropy generations due to magnetic field. It demonstrates that the increase in Rayleigh number for various power-law indexes and Hartmann numbers causes the high values of the entropy generation due to magnetic field to enhance generally. Moreover, it is clear that there are high values of the local entropy generation close to the sidewalls. The maximum values of the local entropy generation due to the magnetic field can exhibit the influence of the Rayleigh number evidently. It also exhibits that the local entropy generation due to magnetic field drops considerably as the power-law index

enhances in multifarious Hartmann numbers and Rayleigh numbers. However, the irreversibility follows the same patterns and shapes for different power-law indexes.

Fig.20 demonstrates the summation local entropy generation ( $S_S$ ) for different Rayleigh numbers, power-law indexes, and Hartmann numbers at  $N_t = N_b = N_r = 0.1$ , and  $Le=1$ . The shape of the total entropy generation at  $Ha=0$  exhibits that the entropy generation due to the fluid friction is dominant in the total irreversibility. However, the increase in Hartmann number causes the shape of the local entropy generation to alter; especially, at  $Ra=10^4$  as the rise of Hartmann number declines the entropy generation due to fluid friction. It is clear that the rise of the Rayleigh number augments the total irreversibility significantly in various Hartmann numbers and power-law indexes. The increase in Hartmann number declines the  $S_S$  where the maximum value of the  $S_S$  drops. This pattern demonstrates that the effect of the entropy generation due to magnetic field is more significant than the irreversibility due to fluid friction.

Fig.21 shows the local Bejan number ( $Be$ ) for different Rayleigh numbers, power-law indexes, and Hartmann numbers at  $N_t = N_b = N_r = 0.1$ , and  $Le=1$ . It shows that the value of the local Bejan number declines generally as the Rayleigh number enhances. The main reason of the trend is the augmentation of the  $S_F$  as the Rayleigh number increases. The maximum value of the local Bejan number in the both studied Rayleigh numbers expands as the power-law index enhances. The increase in Hartmann number declines the maximum value section in the both studied Rayleigh numbers.

Fig.22 indicates the total entropy generations due to heat transfer (ST), fluid friction (SF), mass transfer (SD), the summation of entropy generations (SS), and the average Bejan number for different Hartmann numbers, Rayleigh numbers and power-law indexes at  $N_t = N_b = N_r = 0.1$ , and  $Le=1$ . It indicates that the ST drops gradually as the power-law index enhances for the both Rayleigh numbers while the increase in the Rayleigh number enhances the ST in various power-law indexes and Hartmann numbers. However, the effect of power-law index on ST drops as Hartmann number enhances. The plots exhibit that the SF drops with the rise of the power-law index as the increase in the Rayleigh number enhances the SF considerably. It was found that the SF declines markedly as the Hartmann number increases in the both studied Rayleigh numbers. Moreover, the shear-thinning behaviour diminishes as Hartmann number enhances. The augmentation of power-law index at  $Ha=0$  causes SD to drop in the both studied Rayleigh numbers. At  $Ra=10^4$ , the magnetic field weakens the power-law index influence where SD is nearly the same for different power-law indexes at  $Ha=15$  and  $30$ . In addition, the addition of the magnetic field at  $Ra=10^5$  decreases the SD in various power-law indexes and moreover the power-law index effect drops slightly. At  $Ra=10^5$ ,



the increase in Hartmann number enhances SG significantly while the increase in power-law index declines SG. At  $Ra=10^4$ , the increase in Hartmann number in the power-law indexes of  $0.4 < n < 0.8$  rises SG marginally, but the SG drops with the increase in Hartmann number at  $n=1$ . It is found that total irreversibility (SS) augments substantially with the rise of Rayleigh number in different power-law indexes and Hartmann numbers. In addition, the rise of power-law index diminishes the SS in different Hartmann numbers and Rayleigh numbers. Further, the increase in Hartmann number provokes SS to decline. The average Bejan number drops at  $Ra=10^4$  in the absence of a magnetic field slightly as power-law index augments, but it enhances with the rise of power-law index in the presence of a magnetic field. At  $Ra=10^5$ , the increase of power-law index enhances  $Be_{avg}$  in different Hartmann numbers. In addition, it demonstrates that  $Be_{avg}$  rises from  $Ha=0$  to 15, but the lowest values of  $Be_{avg}$  were observed at  $Ha=30$ .

### 6.6 Effect of Lewis number on entropy generation

Effect of Lewis number on entropy generations due to fluid friction, heat transfer and mass transfer is displayed at Fig.23 where the local total entropy generation and Bejan number provide a clear assessment of the parameter in the figure. The contours of the local entropy generation and maximum values of the entropy generations demonstrate that the augmentation of Lewis number from  $Le=1$  to 10 declines the irreversibilities due to fluid frictions while the entropy generation due to heat transfer enhances marginally. Moreover, entropy generation because of mass transfer is strengthened. In addition, the local Bejan number exhibits that the rise of Lewis number augments the power of the local Bejan number in some sections of the cavity. In fact, high values of irreversibilities are observed in the horizontal sidewalls with the rise of the Lewis number. In addition, the total local entropy generation shows an enhancement with the rise of Lewis number. The comparison between the local Bejan numbers of the Lewis numbers demonstrates that the increase in Lewis number strengthens maximum values in the middle of the cavity. At Fig.24, a comparison between three different Lewis numbers of  $Le=1, 5,$  and 10 has been drawn for different total entropy generations due to heat transfer (ST), fluid friction (SF), mass transfer (SD), the summation of entropy generations (SS), and the average Bejan number for  $N_t = N_b = N_r = 0.1$ ,  $Ha=0$ ,  $Ra=10^5$  and  $n=1$ . It shows that the ST drops from  $Le=1$  to 5 and then increases from  $Le=5$  to 10. The SF decreases steadily as the Lewis number enhances; although, the drop is more significant from  $Le=1$  to 5 compared to the decline from  $Le=5$  to 10. Moreover, the SD, SS, and the average Bejan number augment gradually as the Lewis number increases.

### 6.7 *Effect of Buoyancy ratio number on entropy generation*

The local entropy generations due to fluid friction, heat transfer and mass transfer are displayed in different Buoyancy ratio numbers at Fig.25 where the local total entropy generation and Bejan number also have been displayed. It shows that various entropy generations including the local total entropy generation becomes stronger as the buoyancy ratio number enhances. In addition, it demonstrates that the local Bejan number weakens in different sections in the cavity which clearly exhibits that the enhancement of the Buoyancy ratio number has higher effects on the irreversibility due to fluid friction more than the entropy generations due to heat and mass transfer. The Fig. 26 indicates that the total entropy generations due to heat transfer (ST), fluid friction (SF), mass transfer (SD), and the summation of entropy generations (SS) rise as the Buoyancy ratio number increases. However, the average Bejan number exhibits a different trend where drops significantly when the Buoyancy ratio number enhances.

### 6.8 *Effects of Brownian motion and Thermophoresis parameters on entropy generation*

Effects of Brownian motion and Thermophoresis parameters on the local entropy generations due to fluid friction, heat transfer and mass transfer are exhibited at Fig.27 where the local total entropy generation and Bejan number also have been shown. It indicates that various entropy generations including the local total entropy generation become stronger as the Brownian motion and Thermophoresis parameters enhance. In addition, it shows that the local Bejan number weakens in different sections in the cavity which demonstrates that the enhancement of the Brownian motion and Thermophoresis parameters has higher effects on the irreversibility due to fluid friction more than the entropy generations due to heat and mass transfer. The Fig.28 displays that the total entropy generations due to fluid friction (SF), mass transfer (SD), and the summation of entropy generations (SS) rises as the Brownian motion and Thermophoresis parameters increase. But, the entropy generation due to heat transfer drops from  $N_t = N_b = 0.1$  to  $N_t = N_b = 0.5$  and augments as they rise to  $N_t = N_b = 1$ . In addition, the average Bejan number declines significantly when the Brownian motion and Thermophoresis parameters enhance.

## 7 Concluding Remarks

Entropy generation into natural convection of non-Newtonian nanofluid, using the Buongiorno's mathematical model in a cavity in the presence of a magnetic field has been analyzed by Finite Difference Lattice Boltzmann method (FDLBM). This study has been conducted for the pertinent parameters in the following ranges: the Rayleigh number ( $Ra = 10^4$  and  $10^5$ ), Hartmann numbers ( $Ha = 0, 15, 30$ ), buoyancy ratio number ( $N_r = 0.1, 1, \text{ and } 4$ ), power-law index ( $n = 0.4 - 1$ ), Lewis number ( $Le = 1, 5, \text{ and } 10$ ), Thermophoresis parameter ( $N_t = 0.1, 0.5, 1$ ), and Brownian motion parameter ( $N_b = 0.1, 1, 5$ ). It was found that heat and mass transfer enhance with augmentation of Rayleigh number. The increase in Hartmann number causes heat and mass transfer to drop in different Rayleigh numbers and power-law indexes. Heat and mass transfer alter as the power-law index changes. The heat and mass transfer decline considerably as the power-law index increases at  $Ra=10^5$  in different Hartmann numbers. The influence of the shear-thinning behavior on the nanofluid drops when Hartmann number rises. Heat and mass transfer augment with the increase in the buoyancy ratio number. The enhancement of the Thermophoresis and Brownian motion parameters increases mass transfer while it provokes the heat transfer to drop. The increase in Lewis number enhances mass transfer considerably and declines the heat transfer. It was observed that the enhancement of Rayleigh number augments different irreversibilities and the highest level of growth is observed in the entropy generation due to fluid friction and magnetic field. Bejan number declines significantly with the augmentation of Rayleigh number in different power-law indexes and Hartmann numbers which demonstrates a jump in the irreversibility due to fluid friction. The increase in the power-law index results in the drop of multifarious entropy generations. At  $Ra = 10^5$ , the rise of the power-law index enhances the Bejan number in different Hartmann numbers. It demonstrates that the entropy generations due to fluid friction and magnetic field are more affected against power-law index in comparison with the entropy generations of heat and mass transfer. The rise of Hartmann number declines different entropy generations. In addition, the increase in Hartmann number provokes the power-law index effect to drop significantly. The rise of the power-law index enhances the average Bejan number. The pattern proves that the effect of power-law index on the irreversibility due to the fluid friction and magnetic field is more significant compared to the entropy generation due to heat and mass transfer. The highest values of the average Bejan number is observed at  $Ha=15$  for  $Ra=10^5$ . The rise of the Lewis number enhances entropy generation due to heat transfer and fluid friction while the irreversibility due to the mass transfer and total entropy generation increase. The average Bejan number demonstrates that the increase in the Lewis number results in the drop of the effect of the entropy generation due to fluid friction in the total irreversibility. The enhancement of the buoyancy ratio number provokes the total irreversibility to rise. In other

words, the optimized energy is achieved in lower buoyancy ratios. The total entropy generation increases as the Brownian motion and Thermophoresis parameters augment.

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# Nomenclature

$A_1$	First Rivlin-Ericksen tensor
$B$	Magnetic field
$Be$	Bejan number
$C$	Concentration
$c$	Lattice speed
$c_p$	Specific heat at constant pressure
$D$	Mass diffusivity
$D_B$	Brownian motion
$D_f$	Dufour parameter
$D_T$	Thermophoresis coefficients
$F$	External forces
$f$	Density distribution functions
$f^{eq}$	Equilibrium density distribution functions
$g$	Internal energy distribution functions
$g^{eq}$	Equilibrium internal energy distribution functions
$g_y$	Gravity
$Ha$	Hartmann number
$k$	Thermal conductivity
$L$	Length of the cavity
$Le$	Lewis number
$N_b$	Brownian motion parameter
$N_r$	Buoyancy ratio
$N_t$	Thermophoresis parameter
$Nu$	Nusselt number
$p$	Pressure
$Pr$	Prandtl number
$R$	Gas constant
$Ra$	Rayleigh number
$S_D$	Entropy due to mass transfer
$S_F$	Entropy due to fluid friction
$S_G$	Entropy due to magnetic field
$S_T$	Entropy due to heat transfer
$S_S$	Summation of entropy generations
$Sh$	Sherwood number
$T$	Temperature
$t$	time
$x, y$	Cartesian coordinates
$u$	Velocity in x direction
$v$	Velocity in y direction

## Greek letters

$\beta$	Thermal expansion coefficient
$\phi$	Relaxation time
$\sigma$	Electrical conductivity
$\tau$	Shear stress
$\xi$	Discrete particle speeds
$\Delta x$	Lattice spacing
$\Delta t$	Time increment
$\alpha$	Thermal diffusivity
$\rho_f$	Density of fluid
$\rho_s$	Density of solid
$\eta$	Dynamic viscosity
$\psi$	Stream function value
$II$	Second invariant

### Subscripts

$avg$	Average
$C$	Cold
$H$	Hot
$x, y$	Cartesian coordinates
$\alpha$	Numbers of nodes
$f$	Fluid
$s$	Solid
$T$	Thermal
$tot$	Total
$D$	Solutal

Table 1

Grid independence study at  $Ra = 10^5$ ,  $Ha = 15$ ,  $n=1$ ,  $Le = 1$  and  $Nr=Nt=Nb = 0.1$

Mesh size	$Nu_{avg}$	$Sh_{avg}$
100*100	4.289	1.582
110*110	4.308	0.1.591
120*120	4.428	1.612
130*130	4.491	1.627
140*140	4.528	1.642
150*150	4.536	1.657
160*160	4.536	1.657

Table 2

Comparison of present study with the results of de Vahl Davis [8] for different Rayleigh numbers at  $Pr=0.71$

		Present study	de Vahl Davis [8]
Ra=10 <sup>3</sup>	Nu <sub>avg</sub>	1.118	1.118
	Nu <sub>max</sub>	1.505	1.505
	U <sub>max</sub>	13.644	3.649
	V <sub>max</sub>	3.690	3.697
Ra=10 <sup>4</sup>	Nu <sub>avg</sub>	2.243	2.243
	Nu <sub>max</sub>	3.528	3.528
	U <sub>max</sub>	16.170	16.178
	V <sub>max</sub>	19.613	19.617
Ra=10 <sup>5</sup>	Nu <sub>avg</sub>	4.519	4.519
	Nu <sub>max</sub>	7.717	7.717
	U <sub>max</sub>	34.725	34.730
	V <sub>max</sub>	68.588	68.590