The Effects of Activation Energy and Thermophoretic Diffusion of Nanoparticles on Steady Micropolar Fluid along with Brownian Motion

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1.Introduction

Eringen presented the microfluid theory that describes the mathematical model of the behavior of non-Newtonian fluid, exotic lubricants, polymeric fluids, liquid crystals, ferro liquids, and colloidal fluids [1]. The most important theoretical concept was presented by Eringen using the microfluids, and a famous micropolar fluid (MP) model was introduced [2, 3]. To demonstrate certain microscopic effects, many researchers are taking interest in the micro-rotation and local structure of fluid nanoparticles. Such fluids determined by spin inertia are capable to support the body and stress moments. The theory related to microfluids is not easy to understand due to nontrivial problems [4]. The subclass of microfluids is the MP fluid that involves microrotational effects and microrotational inertia. The MP is a base of the chemical Navier–Stokes model, and the tiny structure of this fluid makes the nature hard to understand. The MP fluid is very important and has vast applications in many industrial processes. Eringen [1] extended the idea to formulate the theory of thermomicropolar fluid. Later on, many researchers studied the following attributes of the edge layer of these fluids over a semi-infinite plate of high temperature. Ishak et al. [5] worked on the flow of the...
stagnation point (SP) over a shrinking sheet using the MP fluid. Ameel et al. [6] used the microchannels to discuss the laminar behavior of the flow using a detailed theory of the MP fluid. Nazar et al. [7] also studied the SP flow of the MP fluid towards the stretching surface. The detail of the boundary layer flow using the MP fluid along with its results is demonstrated by Rees and Bassom [8]. Mitarai et al. [9] worked on the collisional granular flow, which is a type of the MP fluid. Galdi et al. [10, 11] proved that the equations based on the MP fluid can be solved and give unique solutions. A brief study published by the authors proved that the MP fluid equations have unique solutions. Mishra [12] worked on the peristaltic pumping of the MP fluid in a tube and presented numerical results. Particularly, the consequences of MP fluids have been displayed to the theory of lubrication and porous media, see Ref [13–19].

Beg et al. [18] did recent investigation about computation of nonisothermal and thermoconvective micropolar fluid dynamics in a Hall magnetohydrodynamic (MHD) generator system with nonlinear distending wall. Shamshuddin et al. [20] described discussion about micropolar fluid flow, which is induced due to a stretching sheet with heat source/sink and thermosolute chemically reacting micropolar fluid past a permeable stretching porous sheet. Beg et al. [21, 22] found facts about the experimental study of rheology and lubricity of drilling fluids enhanced with nanoparticles, and they published their findings about modeling magnetic nanoparticle flow with induction and nanoparticle solid volume fraction effects. Sheri and Shamshuddin [23] explored the facts about finite element analysis on transient MHD free convective chemically reacting micropolar fluid flow past a vertical porous plate with Hall current and viscous dissipation. Siva and Shamshuddin [24] investigated about transportation of heat in MHD flow along with chemical reaction and viscous dissipation. Shamshuddin et al. [25–27] worked on Lie symmetry analysis and numerical solutions for thermosolutal chemically reacting radiative micropolar flow, finite element computation of multiphysical micropolar transport phenomena from an inclined moving plate in the porous media, and Adomian decomposition method simulation of von Kármán swirling bioconvection nano-fluid flow.

The Brownian motion (BM) is a motion of random particles and plays a vital role in the area of science and biology. The BM is produced due to the continuous bombardment of the molecules in the surrounding medium. This sort of motion is the result of the collision with nearby liquids/gaseous molecules. The mini/microscopic particles suspended in liquids or gases are impacted by the molecules of the fluid covering the particles. Sui et al. [28] studied the transportation of mass, collective motion, and BM. Mendoza-Gonzalez et al. [29] explained the continuous martingales and BM along with the continuity of nanoparticles and transformation of mass. Saffman and Delbruck [30] described the impacts of BM over chemical reactions in the thin sheet of a viscous fluid along with the chemical reactions. Michaelides [31] discussed the nanoparticle suspension during the movement of the liquid. Berla et al. [32] discussed the role of BM, especially in the field of biology. The relation between BM and thermal conductivity is so strong, and by using this fact, Jang and Choi [33] proved that the main cause of BM is the increase in thermal conductivity. The effectiveness of BM can be seen in the references [34–36].

Thermophoresis is the change in position/migration of the large structure molecules to a macroscopic temperature gradient. The phenomenon is observed due to the exhibition of different responses of particles. McNab and Meissen [37] discussed the inspection of thermophoresis in liquids and showed the mixture behavior of nanoparticles. Talbot et al. [38] worked to show the reactions of the mixture of nanoparticles at the heated surface. Piazza and Parola [39] revealed the temperature gradient effects and uses of thermophoresis in colloidal suspensions. Willemsen et al. [40] explored the study of the molecular interaction in microscale thermophoresis. Wienken et al. [41] analyzed the protein binding in biological liquids using microscale thermophoresis. Jerabek-Willemsen et al. [42] presented the comprehensive study about the microscale thermophoresis. Iacopini and Piazza [43] implemented the thermophoresis in proteins. Seidel et al. [44] worked on the quantity of thermophoresis under some challenging conditions of bimolecular interfaces. Jellum et al. [45] discussed the nanoparticle mixture.

The activation energy (AE) is used to proceed exergonic reactions or energy required to initiate the reactions. For this, some or entire chemical linkages in the substrate are broken to form a novel product. The AE does not depend upon the process of exergonic reaction and proceeds in the forward direction/endergonic. The AE would be larger at a constant transition state and needs extra efficient energy to reach the up-hill level of the transition state. The higher the activation energy, the slower the rate of a chemical reaction. In some sort of specific cases at high AE, a reaction does not happen without any input/gain of energy. Sastry et al. [46] discussed distinct dynamical regimes in the energy landscape of a glass-forming liquid. Cohen and Turnbull [47] explored the transport of molecules in both gases as well as liquids. Goldstein [48] worked on the glass transition and viscous liquids using the potential energy. Dey and Bradt [49] discussed the chemical reactions with liquid and thermophoresis. Johari and Goldstein [50] worked on viscous liquids and glass transition. In the industry of chemical engineering, the AE has many uses in the field of geothermal reservoirs, oil emulsions, mechanics of water, and food processing [51–58].

In this work, the effects of MP fluids with BM and thermophoresis are discussed. Moreover, the effect of AE and thermal conductivity is also studied. The equations of motion, angular momentum, temperature, and concentration along with the boundary conditions are listed for the MP fluid. The rest of the paper is organized as follows: Section 2 describes the physical state of the problem. Section 3 presents the designed methodology based on the shooting scheme. Section 4 shows the detailed results and discussions. The conclusions are listed in the last section of the study.
2. Physical Problem Statement

Consider a two-dimensional, incompressible, and steady flow involving mixed convection terms to the MP fluid over a semi-infinite stretching plate with the thermal diffusivity behavior of thermophoresis and BM. The convective surface and ambient temperature of the fluid are \( T_w \) and \( T_{\infty} \), respectively, see Figure 1. The sheet surface and ambient concentrations are \( C_w \) and \( C_{\infty} \), and the flow occupies within the domain \( y > 0 \). Stretchiness of the sheet occurs in the \( x \)-direction by holding the fixed origin, and the \( y \)-axis is perpendicular to it. The \( x \)-axis is taken towards the stretching plate, and the velocity of the sheet in the \( x \)-direction is \( u = u_w(x) = c_1x \). It is assumed that the chemical reaction is induced, and AE initiates the chemical reaction. The properties of the fluid are assumed to be constant in the steady case. Then, under the usual boundary layer approximations, the governing equations of continuity, linear momentum, angular momentum, equation of energy, and concentration are written as follows [59]:

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \tag{1}
\]

\[
\frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + v \frac{\partial^2 u}{\partial y^2} + K_1 \frac{\partial \sigma}{\partial y} + g_1 \beta'' (C - C_{\infty}) + g_1 \beta'' (T - T_{\infty}), \tag{2}
\]

\[
\frac{\partial^2 \sigma}{\partial y^2} - 2 \sigma \frac{\partial u}{\partial y} = 0, \tag{3}
\]

\[
\frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \alpha \frac{\partial^2 T}{\partial y^2} + \tau \left\{ D_T \frac{\partial C}{\partial y} + \frac{D_T}{T_{\infty}} \frac{\partial T}{\partial y} \right\}^2 \tag{4},
\]

\[
\frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = D_T \frac{\partial^2 C}{\partial y^2} + D_T \frac{\partial T}{\partial y} \frac{\partial T}{\partial y} - B_A (T_w - T_{\infty}) w \tag{5},
\]

The boundary conditions are

\[
\begin{align*}
    u &= u_w(x) = c_1 x, \\
    v &= 0, \\
    C &= C_w, \\
    \sigma &= 0, \\
    \frac{\partial T}{\partial y} &= (T_w - T) \text{ at } y = 0, \\
    \psi(x, y) &= \sqrt{c_1 c x} f(\eta), \\
    \theta(\eta) &= \frac{T - T_{\infty}}{T_w - T_{\infty}}, \\
    \phi(\eta) &= \frac{C - C_{\infty}}{C_w - C_{\infty}}, \\
    \sigma &= \sqrt{\frac{\alpha}{v}} x f(\eta), \\
    u &= \frac{\partial \psi}{\partial y} = c_1 x f'(\eta), \\
    v &= \frac{\partial \psi}{\partial x} = -\sqrt{c_1 c} f(\eta), \\
    \eta &= y \sqrt{\frac{c_1}{c}},
\end{align*}
\]

where the stream function is \( \psi \). The transformations (7)–(8) are used in equations (1)–(5). Hence, we get the following system of ODEs:

\[
f'' - f f'' + f' + G_1 g' + G_2 \theta + G_3 \phi = 0, \tag{9}
\]

\[
G g'' - (2 g + f'') = 0, \tag{10}
\]

\[
\theta'' + P \left( f \theta' + N b \theta' \phi' + N t \phi'^2 \right) = 0, \tag{11}
\]
\[ \phi'' + \text{Sc} f'\theta' + \frac{Nt}{Nb} \phi'' = \text{Sc} \lambda^A g'' \exp \left( \frac{-E_a}{\theta} \right) \phi = 0. \] (12)

The boundary conditions become

\[ \begin{align*}
\theta'(0) &= B_i \theta(1 - \theta(0)), \\
f'(0) &= 0, \\
g(0) &= 0, \\
\phi(0) &= 1,
\end{align*} \]

at \( \eta = 0, \)

\[ \begin{align*}
f' &\rightarrow 0, \\
g &\rightarrow 0, \\
\theta &\rightarrow 0, \\
\phi &\rightarrow 0,
\end{align*} \]

as \( \eta \rightarrow \infty. \)

The parameters used in equations (9)–(12) are given as

\[ \begin{align*}
G_1 &= \frac{K_1}{\nu}, \\
G_x &= \frac{g B^* (T_w - T_{\infty})}{c_1 u_w}, \\
G_c &= \frac{g B^{**} (C_w - C_{\infty})}{c_1 u_w}, \\
G &= \frac{G_1 \alpha}{\nu}, \\
Pr &= \frac{\nu}{\alpha}, \\
Nb &= \frac{\tau D_B (T_w - T_{\infty})}{\nu}, \\
Nt &= \frac{D_T (C_w - C_{\infty})}{\nu T_{\infty}}, \\
Sc &= \frac{\nu}{D_B}, \\
\lambda^A &= \frac{\nu B_A (T - T_{\infty})}{c_1}, \\
Ea &= \frac{E_a}{T_w - T_{\infty}}, \\
Bi &= \frac{\frac{\nu}{\sqrt{c_1}}}{\sqrt{c_1}}.
\end{align*} \] (14)

The shear stress and skin-friction coefficient is denoted and defined as:

\[ \tau_w = \left( \mu + \frac{S}{\theta} \right) \frac{du}{dy} \bigg|_{\eta=0}, \]

\[ c_f = \left[ \frac{2 \tau_w}{\rho u^2} \right]_{\eta=0} = -2 \left( \text{Re}_x \right)^{-0.5} f''(0), \]

where \( \text{Re}_x = (c_x/n) \) is the local Reynolds number. From the temperature field, the rate of heat transfer is defined as

\[ q_w = k \left( \frac{\partial T}{\partial y} \right)_{\eta=0}. \] (16)

The coefficient of local heat transfer, local Nusselt number, and couple stress are given as

\[ h(x) = \frac{q_w}{T_w - T_{\infty}}, \]

\[ N_{ux} = \frac{h_x}{k} = (\text{Re}_x)^{-0.5} \theta(0), \]

\[ m_w = G_1 \left[ \frac{\partial \phi}{\partial y} \right]_{\eta=0} = (\text{Re}_x)^{G_1 \alpha} \theta(0). \] (19)

Further, the local mass diffusion flux, local Sherwood number, takes the form as

\[ Sh_x = \frac{x q_m}{D_B (C_w - C_{\infty})}. \] (20)

\[ \frac{Sh_x}{(\text{Re}_x)^{0.5}} = -\phi(0), \] (21)

where \( q_m = -D_B [\partial C/\partial y]_{\eta=0}. \)

The vector form of the skin-friction coefficient, the local Nusselt number, the couple stress number, and the Sherwood number, respectively, is given as

\[ \begin{bmatrix}
\frac{c_f (\text{Re}_x)^{0.5}}{	ext{Re}_x^{0.5}} \\
N_{ux} (\text{Re}_x)^{0.5} \\
\frac{m_w}{G_1 \alpha} (\text{Re}_x)^{-0.5} \\
Sh_x (\text{Re}_x)^{-0.5}
\end{bmatrix} = \begin{bmatrix}
-2 f''(0) \\
\theta'(0) \\
\phi'(0) \\
-\phi'(0)
\end{bmatrix}. \] (22)

### 3. Methodology

In order to present the solution of equations (9)–(12), the shooting scheme is applied [60–63]. The competency of this technique is to shoot the boundary conditions into initial conditions. Four initial conditions using \( f(\eta), g(\eta), \theta(\eta), \) and \( \phi(\eta) \) at \( \eta \rightarrow \infty \) were missing. The use of dummy conditions has been introduced instead of missing conditions. The numerical bvp4c obtained from the concepts
of the finite difference scheme is used to compare the numerical results.

Suppose

\[ y'_1 = y_2, \]
\[ y'_2 = y_3, \]
\[ y'_3 = y_1 y_3 - y'_2 - G_1 y_9 - G_2 y_4 - G_c y_6, \]
\[ y'_4 = y_5, \]
\[ y'_5 = \left[ -Pr(y_1 y_5 - N_b y_7 y_5 - N_t y'_5) \right], \]
\[ y'_6 = y_7, \]
\[ y'_7 = Sc \lambda^A \left( y_4 \right)^w \exp \left( \frac{-E_a}{y_4} \right) y_6 - Sc y_1 y_5 + \frac{N_t}{N_b} y'_5, \]
\[ y'_8 = y_9, \]
\[ y'_9 = \frac{1}{G} \left[ 2 y_8 + y_3 \right]. \]

The concerned initial conditions are

\[ y_1 (0) = y_2 (0) = y_6 (0) = y_8 (0) = 1, \]
\[ y_3 (0) = B_i (1 - y_4 (0)) \text{ at } \eta = 0, \]
\[ y_2 (\eta) \rightarrow 0, \]
\[ y_4 (\eta) \rightarrow 0, \]
\[ y_6 (\eta) \rightarrow 0, \]
\[ y_8 (\eta) \rightarrow 0, \text{ as } \eta \rightarrow \infty. \]

4. Results and Discussion

The detailed results are provided in this section for solving the above system of equations using the shooting technique. The physical quantities related to various parameters are tabulated in Tables 1–3. Table 1 shows the explanation of the Nusselt and Sherwood numbers for the present study. Moreover, the discussions about behavior of local skin friction and couple stress of gas and water using different parameters are described in Tables 2 and 3, respectively. The result shows that by increasing \( Pr \), the Nusselt number gradually increases and the Sherwood number decreases. To increase the BM coefficient, the local Nusselt number gives increasing effects, but the Sherwood number acts opposite to it. To increase the Schmidt number, the opposite behavior is noticed in the case of the Nusselt and Sherwood numbers. To increase the AE parameter, the local Nusselt number and Sherwood number results behave the same, but opposite results are noticed in the case of increasing the local Biot number.

The effects of coupling/interaction constant parameter \( G_s \), Grashof number \( G_r \), concentration of thermal bouncy ratio parameter \( G_c \), microrotation parameter \( G \), Nusselt number \( N_t \), and AE parameter \( E_a \) on the local skin friction and couple stress number for gases as well as for water are presented in Table 2 and 3.

For more investigations, several features based on physical dimensionless parameters are plotted in Figures 2–19 to investigate their physical impact on profiles of velocity, angular velocity, temperature, and concentration. Figure 2 shows the effects of the Grashof number \( G_r \) on the velocity. It is noticed that by increasing the values of \( G_r \), the temperature gradient increases, and due to this fact, the velocity gradient increases. Figure 3 shows the thermal buoyancy ratio parameter \( G_c \) effects on the velocity profile. The velocity increases by increasing the values of \( G_c \). Figure 4 depicts the coupling constant parameter \( G_t \) effects on the velocity profile. As \( G_t \) and coupling constant \( K_i \) are directly related to each other and \( K_i \) is in the flow theory, which determines the relative strength of interaction between particles or fields, so due to this increment in values of \( G_t \), the velocity profile decreases. Figure 5 represents the microrotation parameter \( G \); by increasing the values of \( G \),

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the velocity decreases due to rotation. When the rotation is involved, the linear motion goes down and angular velocity increases. Figure 6 shows that with the greater values of the microrotation parameter $G_t$, angular velocity increases because when the rotation increases, angular velocity also increases. Figures 7–11 indicate the effect of Pr, $Sc$, $Nt$, $Nb$, and $Bi_{\theta}$ on the temperature profile. The Schmidt number $Sc$ is inversely related to the BM parameter. The increase in the values of $Sc$ increases the temperature profile. These results are indicated in Figure 7. Similarly, the Pr values and thermal conductivity are inversely related to each other. The reason is that when Pr increases, the thermal conductivity decreases, and due to this, the temperature profile decreases, as indicated in Figure 8. The observations of the thermophoresis parameter $Nt$ are plotted in Figure 9, and the constant temperature profile decreases by increasing the values of $Nt$. By increasing the value of the BM parameter $Nb$, the random motion of the random particles interacts, and this interaction of these particles becomes the reason of the growing temperature. In Figure 10, the representation of the temperature variation using the values of $Nb$ is presented. The thermal Biot number represents the thermal activity, and it increases by increasing the temperature profile which is also seen in Figure 11.

The effects of $Sc$, Pr, $Nt$, $Nb$, $Bi_{\theta}$, $G_c$, and $\lambda^A$ on the concentration profile are demonstrated in Figures 2–19. It is noticed that by increasing the values of $Sc$ and $Nb$, the concentration profile decreases. Concentration field and its related boundary layer thickness decrease by uplifting the $Sc$ Schmidt number. Actually, this Schmidt number is the ratio of viscosity to mass diffusivity. When the Schmidt number increases, then mass diffusivity decreases and results in reduction in the fluid concentration. Similarly, it is noticed that the nanoparticle concentration field diminishes, and its related concentration boundary layer thickness depreciates by increasing the values of Brownian motion. The Brownian motion takes place due to the presence of nanoparticles and resulted in the depreciation of nanoparticle concentration thickness.
Figures 12–15 represent that by increasing the values of Prandtl number ($Pr$) and Nusselt number ($Nt$), the concentration profile shows increasing behavior. By increasing Prandtl number, the velocity gradient increases, and due to this, the concentration also increases. Similarly, it is concluded that the concentration field enhances by increasing the values of the thermophoresis parameter ($Nt$) because concentration boundary layer thickness is an enhancing function of $Nt$.

Similarly, it is concluded that the concentration field enhances by increasing the values of the thermophoresis parameter ($Nt$) because concentration boundary layer thickness is an enhancing function of $Nt$.

The concentration profile decreases by increasing $Bi_\theta$ because thermal activity decreases with the mass transfer. Figures 16–19 indicate that with the increasing values of $\lambda^A$ and $G_\alpha$, the concentration profile decreases. Concentration increases for $\lambda^A$ due to the Arrhenius function, and $AE$ increases with the reduction of this function.
**Figure 9**: $Nt$ effects on the temperature profile.

**Figure 10**: $Nb$ effects on the temperature profile.

**Figure 11**: $Bi\theta$ effects on the temperature profile.

**Figure 12**: $Sc$ effects on the concentration profile.

**Figure 13**: $Pr$ effects on the concentration profile.

**Figure 14**: $Nt$ effects on the concentration profile.
5. Conclusion

The present study is about to present the effects of activation energy and thermophoretic diffusion of nanoparticles on steady micropolar fluid along with Brownian motion. The designed model is solved using a famous shooting technique. Some root outcomes of the present study are as given in the following:

1. For a greater number of $G_r$, the profile of velocity increases. Increment in $G_r$ means increment in the temperature gradient that causes an increase in the velocity distribution.

2. When there is an increase in the values of the coupling constant parameter $G_1$, the velocity profile decreases.

3. The increasing values of the microrotation $G$ show decrease in the velocity profile due to rotation, and the linear motion decreases and the angular velocity profile increases.

![Figure 15: Nb effects on the concentration profile.](image)

![Figure 18: $G_c$ effects on the concentration profile.](image)

![Figure 16: $B_1b$ effects on the concentration profile.](image)

![Figure 19: $w$ effects on the concentration profile.](image)

![Figure 17: $\Lambda^4$ effects on the concentration profile.](image)
(4) By increasing the value of Nt, the phenomenon of shifting the molecules from one place to another and the boundary layer thickness increase, which cause an increase in the concentration profile.

(5) The temperature profile decreases with enhancing the parameter of thermophoresis Nt. By increasing the values of Nt, the thermal and concentration boundary layer thicknesses are increased, while increasing the BM parameter Nb, the profile of temperature increases.

(6) By increasing the dimensionless AE parameter $\lambda^4$, the nanoparticle concentration profile increases due to the Arrhenius function and AE increases with the reduction of this function.

**Abbreviation**

$K$: Coupling constant
$S$: Constant fluid characteristic
$Ea$: Activation energy coefficient
$K$: Thermal conductivity
$r$: Ratio parameter
$C$: Concentration of the fluid
$T$: Temperature of the fluid
$D_B$: Brownian motion coefficient
$D_T$: Thermophoresis coefficient
$T_\infty$: Infinite temperature
$T_w$: Temperature of the plate
$G_i$: Microrotation constant
$\rho$: Fluid density
$g_1$: Magnitude of the gravity
$\alpha$: Thermal diffusivity
$c_p$: Specific heat
$w$: Constant
$B_0$: Preexponential factor
$G$: Grashof number
$G_c$: Buoyancy ratio parameter
$G$: Microrotation parameter
$Pr$: Prandtl number
$Nb$: Brownian motion parameter
$Nt$: Thermophoresis parameter
$Sc$: Schmidt number
$\lambda^4$: Activation energy parameter
$Bi_0$: Thermal Biot number
$\beta^*$: Thermal expansion coefficient
$\beta^*$: Mass diffusion coefficient
$\nu$: Kinematic viscosity
$c_f$: Skin-friction coefficient
$Re_{ex}$: Local Reynolds number
$Nu_x$: Nusselt number
$m_w$: Couple stress
$Sh_x$: Sherwood number
$\sigma$: Microrotation component.

**Data Availability**

No data were used to support this study.

**Conflicts of Interest**

The authors declare that they have no conflicts of interest.

**References**


