Shape effect of MoS$_2$ nanoparticles on entropy generation and heat transport in viscoelastic boundary layer flow

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Abstract. Due to the unique electro-optical and thermal properties of atomically thin molybdenum disulphide (MoS$_2$), it has the potential to transport excess heat in advanced electronic devices to ensure the efficient working of the device. The present article investigates the impact of adding blade-shaped, brick-shaped, cylinder-shaped and platelet-shaped MoS$_2$ nanoparticles on the heat transport characteristics of viscoelastic ethylene glycol (EG). The time-dependent MHD non-Newtonian nanofluid flow is studied in the presence of temperature- and space-dependent heat source. The influence of different shapes of MoS$_2$ nanoparticles on entropy generation as well as heat transport characteristics of viscoelastic boundary layer flow is studied in depth by plotting comparative graphical profiles. This numerical study will help in achieving the enhancement of heat transfer rate in various industrial processes by opting a suitable nanoparticle shape and adjusting the associated parameters to an appropriate value as suggested by the study.

Keywords. Molybdenum disulphide nanoparticles; shape effect; viscoelastic fluid; entropy; non-uniform heat source/sink.

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1. Introduction

Investigation of heat and mass transfer properties across the boundary layer flow of a non-Newtonian fluid over a stretching sheet or surface is of great significance as it finds immense applications in various engineering processes like extrusion process used for the production of sheets in the polymer industry, to cool down electronic chips or sheets in a quiescent fluid bath etc. The properties of the end product in the extrusion process of a polymer sheet, when it is released from a die can be improved significantly by passing such sheets through various Newtonian or non-Newtonian cooling liquids. The choice of the fluid used in this process has a significant impact on the rate of cooling. Choi et al [1,2] reported that the cooling efficiency of the conventional cooling liquids could be significantly increased by incorporating nanoparticles into them. An exhaustive review on the nanofluid convective heat transfer for different geometries using various approaches and semi-analytical or numerical methods is carried out by Sheikholeslami and Ganji [3]. The heat transfer involved in the boundary layer fluid flow over a stretching sheet with or without nanoparticles is studied by various researchers [4–16].

The shape of the nanoparticles can alter the heat transport characteristics of the nanoliquid to a significant extent. Khan [17] determined the impact of incorporating MoS$_2$ nanoparticles of four different shapes on the heat and flow characteristics of the nanofluid flowing through a vertical porous enclosure. They found that platelet and blade-shaped MoS$_2$ nanoparticles exhibit more rate of heat transport than brick and cylinder-shaped nanoparticles. Alqarni et al [18] examined the influence of suspending MoS$_2$ nanoparticles of different shapes in a nanopolymer gel using a non-Newtonian
fluid model, whereas Khan [17] and Abro et al [19] employed a Newtonian fluid model to determine the impact of incorporating MoS2 nanoparticles of different shapes in water and EG respectively. Khan et al [20] and Abbas et al [21] studied entropy generation by suspending MoS2 and SiO2 nanoparticles in water and propylene glycol, respectively. Their study revealed that MoS2 nanoparticles should be preferred as they affect the flow and heat characteristics more significantly than SiO2 nanoparticles. The numerical investigation by Gireesha et al [22] revealed that cylindrical MoS2 nanoparticles enhance the heat transport more than brick-shaped MoS2 nanoparticles in the case of MoS2–water nanofluid in the presence of thermal radiation. A few more recent numerical investigations discussing the shape effects of MoS2 nanoparticles on heat transport in various cooling fluids are listed in [23–29].

Due to the appreciable temperature difference between the ambient fluid and the sheet surface, it becomes essential to take into account the temperature-dependent heat sources or sinks as they may affect the heat transfer characteristics of the system to a significant level. The impact of internal heat generation on heat transport characteristics of viscous boundary layer flow over stretching sheet was studied by Vajravelu and Hadjini-colau [30,31] using the heat generation relation given by Foraboschi and Federico [32]. Abel et al [33] and Gireesha et al [34] studied numerically the impact of non-uniform heat generation on heat transport characteristics of unsteady MHD boundary layer viscous fluid flow. Their investigations revealed that the effective cooling of the stretching sheet could be achieved by non-uniform heat absorption. Abel and Nandeeppanavar [35] and Bataller [36] explored the influence of non-uniform heat generation on steady viscoelastic boundary layer flow. Sandeep and Sulochana [37] studied the impact of non-uniform heat generation/absorption on unsteady MHD micropolar fluid flow over a shrinking (or stretching) sheet. Anantha Kumar et al [38] and Nagaraja and Gireesha [39] explored the impact of variable heat generation/absorption and exponential space-dependent heat generation, respectively, on heat transport characteristics of MHD Casson fluid flow over a curved stretching sheet. Mahanthesh et al [40] examined the influence of exponential space-dependent heat generation on magnetohydrodynamic nanofluid flow over a disk. Sadiq [41] studied the impact of internal heat source on Cu–water Al2O3–water and TiO2–water nanofluid flow in a thin film over a sheet.

In order to assess the flow and heat transport in fluids like EG, various viscoelastic models have been developed. Though there are several models in the viscoelastic category, grade fluids have their own importance. Second grade fluid models use Rivlin–Erickson tensors in the constitutive stress equation which is widely used by the researchers [42,43] to study the non-Newtonian behaviour of the fluids. A vast literature [44–46] on second grade fluid over stretching sheets is available as this model gives a better prediction on the heat transfer than the viscous models.

Bejan [47] suggested that the available energy in the cooling processes can be optimised by the entropy generation minimisation method. Bejan suggested that a significant part of the energy can be saved by combining thermodynamics with heat transfer and fluid mechanics during the modelling. Various researchers [48–55] have determined the entropy generation rate for viscoelastic fluid flow over a stretching sheet. Marzougui et al [56] and Abdel-Nour et al [57] performed a detailed numerical analysis to evaluate the factors governing the entropy production in MHD convective flow of Cu–water nanofluid and Al2O3–Cu/water hybrid nanofluid, respectively. Mumraiz et al [58] examined the factors governing heat and flow characteristics as well as entropy generation in Al2O3–Cu/H2O hybrid nanofluid flow over stretching sheet while Sheikholeslami et al [59] studied numerically the entropy generation minimisation and heat transport in nanofluid flowing through a circular heat exchanger in order to find the best design for the heat exchanger with lowest entropy production and highest heat transfer rate.

To the best of the author’s knowledge, the impact of incorporating MoS2 nanoparticles of four distinct shapes on heat transport and entropy generation in the unsteady MHD viscoelastic nanofluid boundary layer flow with non-uniform heat generation has not been reported yet. So, a detailed analysis of the entropy generation and heat transport characteristics of EG-based nanofluid with MoS2 nanoparticles of different shapes is carried out. The MHD non-Newtonian nanofluid flow is modelled using a viscoelastic fluid model. The flow governing equations are coupled PDEs of highly nonlinear nature which are solved by shooting strategy along with the Runge–Kutta method. The numerical results are discussed comprehensively to attain a better understanding of the impact of different thermofluidic parameters and nanoparticle shape on the heat and flow characteristics of the nanofluid.

2. Physical and mathematical description of the problem

Consider an incompressible, two-dimensional laminar flow of a viscoelastic nanoliquid over a permeable stretching sheet in an unsteady MHD environment. The nanoliquid comprises MoS2 nanoparticles of a particular shape (blade, brick, cylinder or platelet) immersed in a viscoelastic fluid. The flow is induced by the permeable
sheet stretching with velocity \( u_w(x, t) = ax/(1 - ct) \) in the quiescent surrounding nanofluid. Here \( a, c > 0 \) are constants, and the term \( a/(1 - ct) \) represents the effective stretching rate. Both \( a \) and \( c \) have dimensions of \((\text{time})^{-1}\). The flow region is exposed to the time-varying magnetic field \( B(t) = B_0/\sqrt{1 - ct} \), which is oriented in the positive direction of the Y-axis, as shown in figure 1. The temperature at the surface of the sheet is \( T_w(x, t) = T_\infty + ax^2T_0/2v(1 - ct)^{3/2} \), where \( T_\infty \) and \( T_0 \) are the ambient fluid temperature and constant reference temperature, respectively as specified in Andersson et al [60]. The conservation of mass, momentum and heat equations in the Cartesian coordinates for MHD viscoelastic second grade fluid flow in the presence of heat source/sink are expressed in eqs (1)–(3).

\[
\nabla \cdot \bar{V} = 0
\]

(1)

\[
\rho \left[ \frac{\partial \bar{V}}{\partial t} + (\bar{V} \cdot \nabla)\bar{V} \right] = -\nabla p + \nabla \cdot \tau - \bar{J} \times \bar{B}
\]

(2)

\[
(\rho c_p)_{nf} \left[ \frac{\partial T}{\partial t} + (\bar{V} \cdot \nabla)T \right] = \kappa_{nf} \nabla^2 T + tr(\tau \cdot L) + \frac{\bar{J}^2}{\sigma_{nf}} + Q_s.
\]

(3)

The constitutive stress relation for the viscoelastic second grade fluid is, as stated in eq. (4).

\[
\tau = -pI + A_1 (\mu + \alpha_2 A_1) + \alpha_1 A_2,
\]

(4)

where

\[
A_1 = \nabla \bar{V} + (\nabla \bar{V})^T,
\]

\[
A_2 = \frac{dA_1}{dt} + A_1 \nabla \bar{V} + (\nabla \bar{V})^T A_1,
\]

\[
\mu \geq 0, \quad \alpha_1 \geq 0, \quad \alpha_1 + \alpha_2 = 0,
\]

where \( p \) denotes the hydrostatic pressure, \( \alpha_1 \) and \( \alpha_2 \) are the material moduli, \( \mu \) represents the coefficient of dynamic viscosity, \( pI \) is the hydrostatic pressure, \( \bar{V} \) represents velocity as mentioned in Garg and Rajagopal [42,43]. Further, \( \sigma_{nf} \) denotes the electrical conductivity, \( \bar{J} \) denotes the electrical current and \( \kappa_{nf} \) represents the effective thermal conductivity of the nanofluid. Here \( Q_s \) denotes the heat generation (or absorption) rate per unit volume.

After applying Prandtl’s boundary layer theory as in Schlichting and Gersten [61], for the continuity equation (5) and momentum equation (6), the terms \( \partial^2 u/\partial x^2, \partial u/\partial x, u \) are presumed to be of \( O(1) \) and \( y \) to be \( O(\delta) \) where \( \delta \) denotes the width of the boundary layer as discussed in [62,63].

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

(5)

\[
\rho_{nf} \left( \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) = \mu_{nf} \frac{\partial^2 u}{\partial y^2} + k_1 \left( \frac{\partial^3 u}{\partial y^2 \partial t} + u \frac{\partial^3 u}{\partial x \partial y^2} + v \frac{\partial^3 u}{\partial y^3} \right) + \frac{\bar{J}^2}{\sigma_{nf}} + \frac{Q_s}{\rho_{nf}} u.
\]

(6)

2.1 Heat transport studies

The motive of this investigation is to analyse the effects of shapes of MoS\(_2\) nanoparticles on flow and heat transport characteristics of MoS\(_2\)–EG nanofluid. Heat transport characteristics of MoS\(_2\)–EG for four different shapes of MoS\(_2\) nanoparticles, i.e., blade-shaped, brick-shaped, cylinder-shaped and platelet-shaped MoS\(_2\) nanoparticles, in the viscoelastic carrier fluid are analysed. The energy equation is employed for the same. After applying boundary layer assumptions, the final form of the energy equation with temperature- and space-dependent heat source/sink is given by eq. (7).

\[
(\rho c_p)_{nf} \left( \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = \kappa_{nf} \frac{\partial^2 T}{\partial y^2} + k_1 \left( \frac{\partial u}{\partial y} \frac{\partial^2 u}{\partial y \partial t} + u \frac{\partial^2 u}{\partial x \partial y} + v \frac{\partial^2 u}{\partial y^2} \right) + \mu_{nf} \left( \frac{\partial u}{\partial y} \right)^2 + \sigma_{nf} B^2 u^2 + q'''.
\]

(7)

The temperature- and space-dependent heat generation or absorption term \( q''' \) is modelled as in eq. (8).

\[
q''' = \frac{\kappa f u_w(x, t)}{x v_f} \times \left[ A^*(T_w - T_\infty) \frac{u}{u_w} + B^*(T - T_\infty) \right].
\]

(8)
Table 1. Experimentally determined viscosity coefficients for nanoparticles of distinct sphericity [66].

<table>
<thead>
<tr>
<th>Shape</th>
<th>Blade</th>
<th>Brick</th>
<th>Cylinder</th>
<th>Platelets</th>
</tr>
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<tbody>
<tr>
<td>$\psi$</td>
<td>0.36</td>
<td>0.81</td>
<td>0.62</td>
<td>0.52</td>
</tr>
<tr>
<td>$n$</td>
<td>8.6</td>
<td>3.7</td>
<td>4.9</td>
<td>5.7</td>
</tr>
<tr>
<td>$a'$</td>
<td>14.6</td>
<td>1.9</td>
<td>13.5</td>
<td>37.1</td>
</tr>
<tr>
<td>$b'$</td>
<td>123.3</td>
<td>471.4</td>
<td>904.4</td>
<td>612.6</td>
</tr>
</tbody>
</table>

where $A^*$ and $B^*$ are parameters of space- and temperature-dependent heat source/sink such that $A^*, B^* > 0$ governs internal heat generation while $A^*, B^* < 0$ governs internal heat absorption.

The linear relation given in eq. (9) governs the effective density $\rho_{nf}$ of the nanofluid where $\phi$ represents the volume fraction of MoS$_2$ nanoparticles.

$$\rho_{nf} = (1 - \phi) \rho_f + \phi \rho_p.$$  
(9)

The effective heat capacity of the nanofluid is studied by the linear relation given in eq. (10) as in Xuan and Roetzel [64].

$$(\rho C_p)_{nf} = (1 - \phi) (\rho C_p)_f + \phi (\rho C_p)_p.$$  
(10)

The effective viscosity $\mu_{nf}$ of the nanofluid suspensions, as suggested by molecular dynamic simulations of Rudyak et al [65] is governed by eq. (11).

$$\mu_{nf} = (1 + a' \phi + b' \phi^2) \mu_f.$$  
(11)

The values of the coefficients $a'$ and $b'$ are dependent upon the shape of the nanoparticle. The experimentally determined values of $a'$ and $b'$ (by Timofeeva et al [66]) for the blade-, brick-, cylinder- and platelet-shaped nanoparticles are given in table 1. The effective thermal conductivity of the nanofluid is determined using Hamilton and Crosser model [67].

$$\kappa_{nf} = \frac{\kappa_p + (n - 1) \kappa_f - (n - 1) \phi (\kappa_f - \kappa_p)}{\kappa_p + (n - 1) \kappa_f + \phi (\kappa_f - \kappa_p)} \kappa_f.$$  
(12)

Here $n$ is the shape factor (Das et al [68]) and $n = 3/\psi$ where $\psi$ represents the sphericity. The sphericity $\psi$ values for different shapes of nanoparticles are mentioned in table 1. The effective electrical conductivity of the nanofluid is calculated using Maxwell’s model [17,69].

$$\sigma_{nf} = \left(1 + \frac{3(\sigma_s - \sigma_f) \phi}{(\sigma_s + 2\sigma_f) - (\sigma_s - \sigma_f) \phi} \right) \sigma_f.$$  
(13)

The experimentally determined values of thermal conductivity [70,71], as well as electrical conductivity [72] of MoS$_2$ nanoparticles are given in table 2. Assuming that for $t \leq 0$ no fluid flow occurs, the governing boundary layer equations (5)–(7) will be solved for $t > 0$ by subjecting them to the boundary conditions given by eqs (14) and (15).

$$u = u_w, \quad v = v_w, \quad T = T_w + m_1 \frac{\partial T}{\partial y} \quad \text{at} \quad y = 0 \quad (14)$$

$$u \to 0, \quad T \to T_{\infty}, \quad \frac{\partial u}{\partial y} \to 0 \quad \text{as} \quad y \to \infty. \quad (15)$$

As the governing equations for the prescribed second grade fluid flow are one order higher than that of the Navier–Stokes equation, an additional boundary condition is required for solving the present problem. Here $\frac{\partial u}{\partial y} \to 0$ represents the augmented boundary condition at infinity as the flow is in an unbounded domain (Garg and Rajagopal [43]). Further, $v_w = -v_0 / \sqrt{1 - ct}$ denotes suction or injection velocity depending upon whether $v_w < 0$ or $v_w > 0$. In heat transfer studies, both the Nusselt number and the skin friction coefficient are of engineering importance as they indicate heat transfer rate and the drag at the surface, respectively. The expressions for the Nusselt number ($Nu_x$) and the skin friction coefficient ($C_f$) are given by eq. (16).

$$Nu_x = x q_w / \kappa_f (T_w - T_{\infty}), \quad C_f = \tau_w / \rho_f u_w^2.$$  
(16)

where the expression for the heat flux is given by eq. (17).

$$q_w = -\kappa_{nf} \left( \frac{\partial T}{\partial y} \right)_{y=0}.$$  
(17)

and the wall shear stress given by eq. (18) is considered by following Abbas et al [44].

$$\tau_w = \left( \frac{\mu_{nf}}{\partial y} \right)_{y=0} + k_1 \left( \frac{\partial^2 u}{\partial y^2} + u \frac{\partial^2 u}{\partial x \partial y} + 2 \frac{\partial u}{\partial x} \frac{\partial u}{\partial y} + \frac{\partial^2 u}{\partial y^2} \right)_{y=0}.$$  
(18)

3. Solution process

The solution process of the governing partial differential equations (5)–(7) subject to the boundary conditions (14) and (15) consists of two parts. In the first part, we convert PDEs (partial differential equations) governing the flow to ordinary differential equations (ODEs) with the help of similarity transformations. In the second part, we solve the resulting ODEs numerically using the fourth-order Runge–Kutta method along with the shooting strategy.

3.1 Non-dimensionalisation

The coupled PDEs (5)–(7), which are of highly nonlinear nature along with the boundary conditions (14) and (15) are transformed to the set of non-dimensional coupled ODEs by making use of similarity transformations and stream function $\psi$. In accordance with the continuity equation, the stream function must satisfy
Here, \( \psi \), \( \theta \), \( f \), \( \phi \), \( \kappa \), and \( \sigma \) are non-dimensional quantities where prime symbolises the differentiation with respect to \( \eta \). Further, the non-dimensional numbers involved in this process are:

\[
\begin{align*}
S & = \frac{v_0}{\sqrt{\nu}} \\
\text{Pr} & = \frac{\mu_f (c_p)_f}{\kappa_f} \\
\text{Ec} & = \frac{u_w^2}{(c_p)_f (T_w - T_\infty)} \\
\text{} & = \frac{\mu_f (c_p)_f}{\kappa_f} \\
M & = \sqrt{\frac{\sigma}{\rho_f a}} B_0 \\
\end{align*}
\]

is the suction/injection parameter, is Prandtl number, is the unsteadiness parameter, is second grade fluid parameter, is thermal slip parameter and is the magnetic number.

The constants \( A_1 \), \( A_2 \), \( A_3 \) and \( A_4 \) are defined as in eq. (25).

\[
\begin{align*}
A_1 &= \frac{\rho_{nf}}{\rho_f}, \quad A_2 = \frac{(\rho c_p)_{nf}}{(\rho c_p)_f}, \\
A_3 &= \frac{k_{nf}}{\kappa_f}, \quad A_4 = \frac{\sigma_{nf}}{\sigma_f}. \\
\end{align*}
\]

After non-dimensionalisation, the Nusselt number and the skin-friction coefficient are expressed as

\[
\begin{align*}
Nu_r &= Nu_x Re_x^{-1/2} = -\frac{k_{nf}}{\kappa_f} \theta'(0) \\
C_{fr} &= C_f Re_x^{1/2} = \left( \frac{\mu_{nf}}{\mu_f} f''(\eta) \\
&\quad + b^*(3 f'(\eta) f'''(\eta) + \frac{A}{2} (\eta f''''(\eta) + 3 f'''(\eta)) \right) \\
&\quad - f(\eta) f''''(\eta) \big|_{\eta=0},
\end{align*}
\]
where $Nu_r$ represents the reduced local Nusselt number, $C_{fr}$ represents the reduced skin friction coefficient and $Re_x = U_0 x / v_f = ax^2 / v_f(1 - ct)$ is the local Reynolds number. So, apart from the temperature investigation are the reduced Nusselt number $Nu_r$ and the reduced skin-friction coefficient $C_{fr}$.

3.2 Numerical solution

For finding the solution of highly nonlinear ODEs numerically, the immediate step after non-dimension- alisation is to transform them into a system of first-order ODEs. The nonlinear ODEs obtained in the last section are converted to the first-order ODEs by using the substitution provided by eq. (28).

\[
\begin{align*}
(f, f', f'', \theta, \theta') &= (y_1, y_2, y_3, y_4, y_5, y_6) \\
\frac{dy_1}{d\eta} &= y_2, \quad \frac{dy_2}{d\eta} = y_3, \quad \frac{dy_3}{d\eta} = y_4, \quad \frac{dy_4}{d\eta} = \frac{1}{\frac{y_1}{2} + \frac{A}{2} \eta + \frac{A}{2} \phi + b \phi^2} \\
&\quad \times \left( 1 + a \phi + b \phi^2 \right) y_4 \\
&\quad - A_1 \left( y_2^2 - y_1 y_3 + A (y_2 + \frac{\eta}{2} y_3) \right) \\
&\quad + b^* (2 y_2 y_4 - y_2^2 + 2 A y_4) - A_4 M^2 y_2 \\
\frac{dy_5}{d\eta} &= y_5, \quad \frac{dy_6}{d\eta} = \frac{Pr A_2}{A_3} \left\{ 2 y_5 y_2 - y_1 y_5 + A \frac{2}{2} (3 y_5 + \eta y_6) \right\} \\
&- \frac{M^2 Ec Pr A_4}{A_3} \left( \frac{1}{2} + a \phi + b \phi^2 \right) Pr Ec \frac{A}{A_3} y_5^2 \\
&- \frac{1}{A_3} \left( A^* y_2 + B^* y_5 \right) - b^* \frac{Pr Ec}{A_3} y_2 y_5 \\
&\quad \left\{ \frac{A}{2} \left( \eta y_3 y_4 + 3 y_5^2 \right) + y_2 y_3^2 - y_1 y_3 y_4 \right\}.
\end{align*}
\]

The transformed form of the boundary conditions in terms of $(y_1, y_2, y_3, y_4, y_5, y_6)$ is

\[
\begin{align*}
y_1(0) &= S, \quad y_2(0) = 1, \quad y_5(0) = 1 + d_1 y_6(0) \quad (30) \\
y_2(\infty) &= 0, \quad y_3(\infty) = 0, \quad y_5(\infty) = 0. \quad (31)
\end{align*}
\]

The above system of equations (eqs (29)–(31)) is solved by the fourth-order Runge–Kutta method along with the well-known shooting strategy. To integrate the system of the first-order ODEs given in (29), the initial guess values $s_1$, $s_2$ and $s_3$ are chosen to have the set of initial conditions at $\eta = 0$ as given by eq. (32).

\[
\begin{align*}
y_1(0) &= S, \quad y_2(0) = 1, \quad y_3(0) = s_1, \quad y_4(0) = s_2, \quad y_5(0) = s_3, \quad y_5(0) = 1 + d_1 y_6(0).
\end{align*}
\]

After choosing the initial guess values $s_1$, $s_2$ and $s_3$, the initial value problem given by eqs (29) and (32) is integrated using the Runge–Kutta method till $\eta_\infty$. The initial guess values $s_1$, $s_2$ and $s_3$ are chosen respectively for the unknowns $y_3(0)$, $y_4(0)$ and $y_5(0)$ as Runge–Kutta fourth-order method requires all the values $y_1(0)$, $y_2(0)$, ..., $y_5(0)$ at $\eta = 0$ to integrate the system of equations till $\eta_\infty$. The choice of $\eta_\infty$ is taken to be a large value such that the temperature profiles are asymptotic in nature. Now, when eq. (29) is solved with the shooting method using the initial conditions mentioned in eq. (32), then the computed boundary values at $\eta_\infty$ depend upon the choice of the initial guess values $s_1$, $s_2$ and $s_3$. The correct choice of $s_1$, $s_2$ and $s_3$ yields the given boundary conditions at $\eta_\infty$. A system of algebraic equations is thus formulated by equating the results obtained for $y_2$, $y_3$ and $y_5$ at $\eta_\infty$ through numerical integration to the actual values given by the boundary conditions in eq. (31), which are further solved using the Newton–Raphson method (Jaan Kiusalaas [73]). While obtaining the solution of the above system of ODE’s, one has to choose the required initial guesses very carefully as a reasonably good guess is needed to ensure the desired error tolerance, while obtaining a solution as a bad guess would lead to a singular Jacobian matrix.

3.3 Code verification

A MATLAB code is developed to obtain the numerical solution using the numerical scheme mentioned in the last section. The accuracy of the code is checked before using it by verifying the results obtained using the same against that of the already published results for the limiting case, as shown in table 3. The validation is performed by comparing the values of $-\theta'(0)$ obtained using the present code with the ones in Grubka and Bobba [4] (Kummer’s function series solution) for the steady viscous case without suction/injection by taking $M = 0$, $S = 0$, $b^* = 0$, $A = 0$, $\phi = 0$ and Ishak et al [6] (Keller box method) for the unsteady viscous case with suction/injection by taking $M = 0$, $b^* = 0$, $\phi = 0$, $A = 0$, $S = 1.5$, $0$, $1.5$ in the governing equations. The calculated results are in perfect harmony with the already published literature, as can be seen from table 3. It was observed during code verification that a fair initial guess and an appropriate value of $\eta$ at infinity would lead to the faster convergence of the solution, and a bad guess can lead to a singularity in the
Table 3. Resemblance of $-\theta'(0)$ with the already published results for code verification.

<table>
<thead>
<tr>
<th>$A$</th>
<th>Pr</th>
<th>$S$</th>
<th>$-\theta'(0)$</th>
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</thead>
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<tr>
<td>0</td>
<td>0.72</td>
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<td>0</td>
<td>1.3205</td>
<td>1.3206</td>
</tr>
<tr>
<td></td>
<td>1.5</td>
<td>2.2224</td>
<td>2.2224</td>
</tr>
</tbody>
</table>

Jacobian iterations. So, while obtaining the results, one should be very careful in choosing an initial guess.

4. Entropy generation analysis

In various industrial and engineering processes, entropy generation destroys the available energy of the system. Therefore, it becomes essential to determine the entropy production rate in a system in order to avoid the wastage of useful energy. The volumetric rate of local entropy generation for MHD viscoelastic nanofluid flow is accounted for by eq. (34) in [48,74–76].

\[
S_{gen} = \kappa_{nf} \left( \frac{\partial T}{\partial y} \right)^2 \frac{\mu_{nf}}{T_\infty} \left( \frac{\partial u}{\partial y} \right)^2 + \frac{k_1}{T_\infty} \left( \frac{\partial u}{\partial y} \frac{\partial^2 u}{\partial y \partial t} + \frac{\partial \phi}{\partial x} \frac{\partial u}{\partial y} + \frac{\partial^2 u}{\partial y^2} \frac{\partial u}{\partial x} \right) \frac{T_\infty}{\sigma_{nf} B^2 u^2}.
\] (35)

The dimensionless entropy generation number is defined as

\[
N_S = \frac{S_{gen}}{S_o},
\]

where $S_o$ is the characteristic entropy generation rate which for prescribed boundary condition is defined as

\[
S_o = \frac{\kappa_f (T_w - T_\infty)^2}{T_\infty^2 x^2}.
\]

So, the non-dimensional form of local entropy production can be written as

\[
N_S = N_H + N_F + N_M,
\] (36)

where $N_H$, $N_F$ and $N_M$ denotes the dimensionless form of local entropy generation due to heat transfer, fluid friction and Joule dissipation, respectively. The descriptive form of non-dimensional entropy production rate after applying similarity transformations is
5. Results and discussions

The motive of this investigation is to analyse the shape effects of MoS$_2$ nanoparticles on heat transport characteristics of MoS$_2$–EG nanofluid. The influence of pertinent parameters like Prandtl’s number, second grade viscoelastic fluid parameter, magnetic number, Eckert number, unsteadiness parameter and heat source/sink parameter on the temperature field, heat transfer rate, entropy generation number and skin friction for four different shapes of MoS$_2$ nanoparticles, i.e., blade-shaped, brick-shaped, cylinder-shaped and platelet-shaped MoS$_2$ nanoparticles suspended in viscoelastic EG are investigated in detail. A comparative analysis giving an insight into the entropy production, skin friction and heat transport characteristics of MoS$_2$–EG nanofluid is carried out for distinct shapes of MoS$_2$ nanoparticles. The numerical results are computed by assigning the values $Ec = 0.4$, $\phi = 0.06$, $b^* = 1$, $Pr = 51$, $A = 0.1$, $A^* = B^* = 0.1$, $Re = 1$, $\Omega = 1$, $M = 1$, $S = 2$ to the parameters unless otherwise specified in the graphs.

5.1 Effect on temperature and entropy production in the boundary layer

The impact of varying Eckert number on temperature profiles of MoS$_2$–EG nanofluid corresponding to MoS$_2$ nanoparticles of four different shapes is presented in figure 2a. The temperature increases for all four nanofluids with an increment in Eckert number. The following trend is observed in temperature profiles near the sheet surface among four nanofluids with different shapes of nanoparticles:

$T_{\text{Blade}} < T_{\text{Brick}} < T_{\text{Cylinder}} < T_{\text{Platelet}}$.

Figures 2b, 3, 4 and 5 present respectively the influence of $Ec$, $A$, $b^*$ and $M$ on the MoS$_2$–EG nanofluid.
Figure 3. Influence of \( A \) on the temperature profile of MoS\(_2\)–EG nanofluid with the blade-shaped MoS\(_2\) nanoparticles.

Figure 4. Influence of \( b^* \) on the temperature profile of the nanofluid with blade-shaped MoS\(_2\) nanoparticles.

Figure 5. Influence of \( M \) on the temperature profile of the nanofluid with blade-shaped MoS\(_2\) nanoparticles.

Figure 6. Influence of heat generation/absorption on the temperature profiles of MoS\(_2\)–EG nanofluid for distinct shapes of MoS\(_2\) nanoparticles.

Figure 7. Influence of Prandtl number on the temperature profile of MoS\(_2\)–EG nanofluid for four different shapes of MoS\(_2\) nanoparticles.

with blade-shaped MoS\(_2\) nanoparticles. These figures depict that an increment in \( Ec, b^* \) or \( M \) results in the enhancement of nanofluid temperature, but an increment in unsteadiness parameter reduces the nanofluid temperature. Similar behaviour was observed for the remaining three shapes during numerical computations. The nanofluid temperature is enhanced within the boundary layer by an increment in Eckert number \( Ec \), the magnetic number \( M \) and viscoelastic fluid parameter \( b^* \). Actually, an increment in \( b^* \) leads to the thickening
of the thermal boundary layer, and a larger value of $Ec$ or $M$ offers more resistance to the nanofluid motion leading to enhanced nanofluid temperature. Figures 6 and 7 show the impact of heat source/sink parameter and Pr respectively on the temperature profiles of MoS$_2$–EG nanofluid corresponding to four different shapes of MoS$_2$ nanoparticles. Figures 6 and 7 reveal that for a fixed value of heat source/sink parameter or Pr, the nanofluid temperature near the sheet surface is minimum for the nanofluid with blade-shaped MoS$_2$ nanoparticles and is maximum for the nanofluid with platelet-shaped MoS$_2$ nanoparticles. The following trend in the nanofluid temperature is observed at a particular value of Pr among four distinct shaped nanoparticles in EG:
Further, figure 7 implies that the nanofluid temperature drops down with an increment in Pr. It happens because the rate of thermal diffusion drops down with an increment in Pr. Figure 8 shows the shape effect of MoS$_2$ nanoparticles on entropy generation rate in MoS$_2$–EG nanofluid. The entropy generation number for MoS$_2$–EG nanofluid is minimum when the MoS$_2$ nanoparticles are of blade shape while it is maximum with the platelet-shaped MoS$_2$ nanoparticles. Figure 8 also reveals that the entropy production is maximum at the sheet surface, and it goes asymptotically to zero towards the edge of the boundary layer. It is quite evident as the values of $f$, $f'$ or $\theta$ vanish asymptotically as $\eta$ approaches infinity. The following trend is observed in the entropy generation number $N_S$ among the four nanofluids corresponding to different shapes of the nanoparticles:

$T_{\text{Blade}} < T_{\text{Brick}} < T_{\text{Cylinder}} < T_{\text{Platelet}}$.

Figures 9–12 represent respectively the influence of $Ec$, $M$, $b^*$ and $A$ on entropy generation rate for the nanofluid with blade-shaped nanoparticles. The value of $N_S$ enhances with an increment in $Ec$ or $M$, whereas it decreases with an increment in $b^*$ or $A$. Physically, an upsurge in $Ec$ enhances the fluid friction between the adjacent layers of the nanofluid, which in turn raises the value of $N_S$ as $N_S$ is an increasing function of dissipative forces. An enhancement in entropy generation number by enhancing magnetic number $M$ implies that the presence of magnetic field leads to entropy generation in the nanofluid. Physically, a larger $M$ offers more resistance to the nanofluid flow resulting
in enhancing heat in the system and thus rising $N_S$. Figures 11 and 12 imply that the entropy generation rate can be reduced significantly by increasing viscoelastic fluid parameter $b^*$ or unsteadiness parameter $A$. A similar trend was observed for entropy generation profiles of MoS$_2$–EG nanofluid with the other shapes of MoS$_2$ nanoparticles during the numerical computations.

5.2 Effect on Nusselt number and skin friction at the surface

The variation in Nusselt number ($Nu$) with unsteadiness parameter $A$ and magnetic number $M$ for MoS$_2$–EG nanofluid with brick-shaped MoS$_2$ nanoparticles is illustrated in figure 13a while a comparative view among the $Nu$ profiles for the four nanofluids (i.e., for brick-shaped MoS$_2$ in EG, blade-shaped MoS$_2$ in EG, cylinder-shaped MoS$_2$ in EG and platelet-shaped MoS$_2$ in EG) is presented in figure 13b. Clearly, an increment in $M$ reduces the magnitude of $Nu$ while an increment in $A$ enhances it. This is because an increment in $M$ makes the thermal boundary layer thicker, while an increment in $A$ reduces the width of the thermal boundary layer (figures 3 and 5). Similarly, figure 14a illustrates the influence of $Ec$ on $Nu$ for the nanofluid with brick-shaped nanoparticles, while figure 14b shows the same for the four distinct nanofluids corresponding to four shapes of MoS$_2$ nanoparticles. Figures 15a and 15b imply that an increment in heat source parameters $A^*$ and $B^*$ augment the magnitude of $Nu$ for all four nanofluids. It can be depicted from figures 13b, 14b and 15b that the magnitude of $Nu$ (i.e., heat transfer rate) is maximum for the nanofluid with platelet-shaped MoS$_2$ nanoparticles but least with brick-shaped MoS$_2$ nanoparticles. It implies that the shape of nanoparticle plays a significant role in heat transport.
Figure 17. Impact of $M$ and $A$ on (a) skin-friction profile of MoS$_2$–EG nanofluid with blade-shaped MoS$_2$ nanoparticles and (b) skin-friction profiles of MoS$_2$–EG nanofluid for four distinct shapes of MoS$_2$ nanoparticles.

Figures 16a, 17a and 18a show the impact of increment in $A$, $b^*$, $M$ and $Ec$ on skin-friction coefficient profiles for blade-shaped MoS$_2$ nanoparticles in EG. However, figures 16b, 17b and 18b give a comparative view among the skin-friction (Sf) profiles of the four nanofluids with variation in thermofluidic parameters $A$, $b^*$, $M$ and $Ec$. The sign of skin-friction coefficient is negative for all the four nanofluids. A hike in the magnitude of skin-friction coefficient is observed with an increment in $A$, $b^*$, $M$ or $Ec$. The following trend is noticed in the magnitude of skin-friction coefficient for different shapes of MoS$_2$ nanoparticles in EG:

$$(Sf)_{\text{Blade}} < (Sf)_{\text{Brick}} < (Sf)_{\text{Cylinder}} < (Sf)_{\text{Platelet}}.$$  

Among the four shapes, the nanofluid with platelet-shaped MoS$_2$ nanoparticles encounter the maximum magnitude of skin friction while the one with blade-shaped MoS$_2$ nanoparticles experiences the least. This implies that not only the heat transport characteristics but the fluid flow characteristics of the nanofluid are also affected deeply by the choice of nanoparticle shape.

6. Conclusions

The influence of shape of MoS$_2$ nanoparticles on EG-based MHD non-Newtonian nanofluid flow is studied in the presence of temperature- and space-dependent heat source. A comparative analysis among different shapes of MoS$_2$ nanoparticles, giving an insight into the heat transport characteristics and entropy production rate of the MoS$_2$–EG nanofluid, is carried out. Significant findings of the analysis are listed as follows:

- The nanofluid temperature in the boundary layer is maximum with platelet-shaped nanoparticles but least with blade-shaped nanoparticles.
- A drop in nanofluid temperature is experienced by an upsurge in unsteadiness parameter or Pr, whereas
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