



# Numerical simulation for aspects of homogeneous and heterogeneous reactions in forced convection flow of nanofluid



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## ARTICLE INFO

### Article history:

Received 17 May 2017

Received in revised form 26 October 2017

Accepted 30 November 2017

Available online 6 December 2017

### Keywords:

Mixed convection

Stagnation point flow

Homogeneous-heterogeneous reactions

Nanofluids

## ABSTRACT

Mixed convection stagnation point flow of nanofluid by a vertical permeable circular cylinder has been addressed. Water is treated as ordinary liquid while nanoparticles include aluminium oxide, copper and titanium dioxide. Homogeneous-heterogeneous reactions are considered. The nonlinear higher order expressions are changed into first ordinary differential equations and then solved by built-in-Shooting method in mathematica. The results of velocity, temperature, concentration, skin friction and local Nusselt number are discussed. Our results demonstrate that surface drag force and heat transfer rate are enhanced linearly for higher estimation of curvature parameter. Further surface drag force decays for aluminium oxide and it enhances for copper nanoparticle. Heat transfer rate enhances with increasing all three types of nanoparticles. In addition, the lowest heat transfer rate is obtained in case of titanium dioxide when compared with copper and aluminium oxide.

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## Introduction

Many industrial liquids have low thermal conductivity which limits the quality of final product during engineering procedure. Pioneer concept of nanomaterial with improved thermal conductivity was given by Choi [1]. Nanotechnology has significance in atomic reactors, chemical process, energy process, mechanical cooling, indicative tests, extraction of geothermal force, disease treatment, heat exchangers and some applications in micro scale fluidic. Convective transport in nanofluids subject to thermophoresis and Brownian effects is explored by Bouniorno [2]. Effect of nanomaterials on natural convective flow past a vertical surface is examined by Kuznetsov and Nield [3]. Later on the same problem is discussed by Nield and Kuznetsov [4] for a porous space. MHD natural convection carbon nanotubes flow has been studied by Ellahi et al. [5]. Nanofluid flow of forced convection with magnetic field utilizing LBM is explored by Sheikholeslami et al. [6]. Convective heat transfer characteristics of Al<sub>2</sub>O<sub>3</sub> nanomaterials submerged in water is studied by Hwang et al. [7]. Kumaresan et al. [8] discussed convective heat transfer characteristics of secondary refrigerant based nanofluids. Flow of nanofluid in a porous channel is addressed by Hatami et al. [9]. Farooq et al. [10] analyzed MHD stagnation point flow of Jeffrey nanomaterial in the presence

of radiation. Mabood et al. [11] addressed mixed convection unsteady flow of nanofluid with viscous dissipation. Convective flow of Cu-water nanomaterial by a rotating cone using is studied by Dinarvand and Pop [12]. Few more recent studies about flows of nanofluids can be visualized through the attempts [13–18].

Heat transfer in flow over a stretchable surface has widespread applications. Due to tremendous applications in engineering and sciences, a large amount of work is focussed at present in this area, drawing of plastic sheets, fibres glass, paper production, metal spinning, fibre and wire coating, food stuff processing, continuous casting, exchangers and chemical processing equipment. All procedures of coating involve a smooth glossy surface to fulfill the necessities for appearance, transparency, strength and low fraction. Crane [19] initiated flow of viscous liquid by a stretched surface. MHD stagnation point flow of rate type nanofluid with thermophoresis is investigated by Bai et al. [20]. Heat transfer in flow of micropolar liquid over a porous stretching surface is examined by Turkyilmazoglu [21]. Melting heat transfer and homogeneous heterogeneous reactions in MHD viscous liquid flow by a stretchable surface is explored by Hayat et al. [22]. Magnetohydrodynamic nanofluid flow past a porous plate with radiation, chemical reaction and rotation is considered by Reddy et al. [23]. Consequences of convective boundary conditions and chemical reaction on flow due to a plate are considered by Rout et al. [24]. Application of non-Fourier heat flux in flow of Jeffrey liquid with temperature dependent thermal conductivity is studied by Hayat

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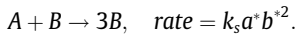
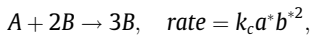
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et al. [25]. Hayat et al. [26] also investigated chemically reactive flow and non-Fourier heat flux in flow by a stretching surface. Viscous dissipation in three dimensional flow of viscous nanofluid is reported by Mahanthesh et al. [27]. Numerical simulation is performed in this work. Hayat et al. [28] examined flow of Burgers nanofluid in presence of magnetohydrodynamics (MHD) and convective condition. Li et al. [29] discussed characteristics of non-Fourier heat conduction in MHD nanofluid flow by a stretched surface. Stretched flow of Oldroyd-B fluid with Cattaneo-Chrisitov heat flux is inspected by Hayat et al. [30].

Prime objective of this analysis is to analyze the impacts of thermal radiation and mixed convection in stagnation point flow of viscous nanofluid by a vertical permeable cylinder. Homogeneous-heterogeneous reactions are also accounted. Induced electric and magnetic fields are absent. Computations for strong nonlinear systems are presented after non-dimensionalization through built-in-Shooting method [31–35]. Graphical analysis for various influential variables is addressed in detail.

**Formulation**

We investigate the mixed convection stagnation point flow of an electrically conducting incompressible viscous nanofluid by a vertical permeable circular cylinder of radius  $a$ . We choose cylindrical coordinate system such that  $x$  is along the stretching cylinder and  $r$  normal to  $x$ . Here  $u$  and  $w$  are the velocity components in  $x$  and  $r$  directions (see Fig. 1). A magnetic field of strength  $B_0$  is exerted along radial direction. We represent  $T_w$  as temperature of cylinder and  $T_\infty$  the ambient temperature. For the formation of compound  $3B$  the fluid phase reaction is [22,26]:



In above expressions  $A$  and  $B$  denote chemical species,  $a^*$  and  $b^*$  the concentrations and  $k_c$  and  $k_s$  the rate constants. Both reaction processes are isothermal. The subjected problems statements are

$$\frac{\partial(ru)}{\partial x} + \frac{\partial(rw)}{\partial r} = 0, \tag{1}$$

$$u \frac{\partial u}{\partial x} + w \frac{\partial u}{\partial r} = u_e \frac{du_e}{dx} + \nu_{nf} \left( \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} \right) + \frac{\sigma_{nf} B_0^2}{\rho_{nf}} (u_e - u) + \frac{\phi \rho_s \beta_s + (1 - \phi) \rho_f \beta_f}{\rho_{nf}} g(T - T_\infty), \tag{2}$$

$$u \frac{\partial T}{\partial x} + w \frac{\partial T}{\partial r} = \alpha_{nf} \left( \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right), \tag{3}$$

$$u \frac{\partial a^*}{\partial x} + w \frac{\partial a^*}{\partial r} = D_A \left( \frac{\partial^2 a^*}{\partial r^2} + \frac{1}{r} \frac{\partial a^*}{\partial r} \right) - k_c a^* b^{*2}, \tag{4}$$

$$u \frac{\partial b^*}{\partial x} + w \frac{\partial b^*}{\partial r} = D_B \left( \frac{\partial^2 b^*}{\partial r^2} + \frac{1}{r} \frac{\partial b^*}{\partial r} \right) + k_c a^* b^{*2}. \tag{5}$$

with

$$u = u_w(x) = u_0 \left( \frac{x}{l} \right), \quad w = V_w^*, \quad T = T_w(x) = T_\infty + \Delta T \left( \frac{x}{l} \right),$$

$$D_A \frac{\partial a^*}{\partial r} = k_s a^*, \quad D_B \frac{\partial b^*}{\partial r} = -k_s a^* \text{ at } r = a,$$

$$u \rightarrow u_e(x) = u_\infty \left( \frac{x}{l} \right), \quad T \rightarrow T_\infty, \quad a^* \rightarrow a_0, \quad b^* \rightarrow 0 \text{ when } r \rightarrow \infty. \tag{6}$$

In above equations  $u$  and  $w$  indicate the velocity components,  $u_e$  the free stream velocity, where  $V_w^* < 0$  corresponds to suction and  $V_w^* > 0$  for injection,  $u_w$  the stretching velocity,  $\nu_{nf}$  the kinematic viscosity,  $T$  the temperature,  $T_\infty$  the ambient temperature,  $\rho_f$  the density of nanofluid,  $g$  the gravity acceleration,  $\phi$  the nanoparticle volume fraction,  $\beta$  the thermal expansion coefficient,  $a^*$  and  $b^*$  the concentrations,  $l$  the characteristics length,  $B_0$  the uniform magnetic field,  $\sigma$  the electrical conductivity,  $D_A$  and  $D_B$  the diffusion species,  $a_0$  the positive dimensional constant,  $k_s$  the heat transfer coefficient,  $\beta$  the coefficient of thermal expansion and  $\alpha_{nf}$  thermal diffusivity. Their definitions are

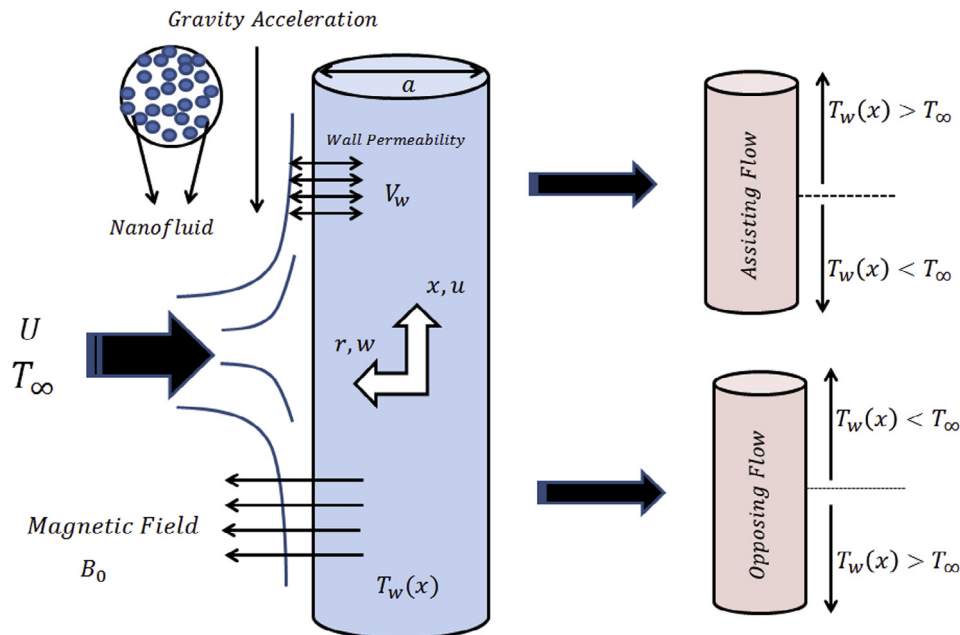


Fig. 1. Flow configuration.

$$v_{nf} = \frac{\mu_f}{(1 - \phi)^{2.5}[(1 - \phi)\rho_f + \phi\rho_s]}, \tag{7}$$

$$\rho_{nf} = (1 - \phi)\rho_f + \phi\rho_s, \tag{8}$$

$$\alpha_{nf} = \frac{k_{nf}}{(\rho C_p)_{nf}}, \tag{9}$$

$$(\rho C_p)_{nf} = (1 - \phi)(\rho C_p)_f + \phi(\rho C_p)_s, \tag{10}$$

$$\frac{k_{nf}}{k_f} = \frac{(k_s + 2k_f) - 2\phi(k_f - k_s)}{(k_s + 2k_f) + \phi(k_f - k_s)}, \tag{11}$$

in which  $\phi$  nanoparticle volume fraction,  $\rho_f$  and  $\rho_s$  density of fluid and solid particles,  $\mu_f$  dynamic viscosity of fluid and  $k_f$  and  $k_{nf}$  thermal conductivities of fluid and nanomaterial respectively. **Table 1** Having transformations

$$\eta = \frac{r^2 - a^2}{2lv_f} \left( \frac{U_\infty lv_f}{a^2} \right)^{\frac{1}{2}}, \quad \psi = \left( \frac{U_\infty v_f a^2}{l} \right)^{\frac{1}{2}} x f(\eta), \quad u = \left( \frac{1}{r} \right) \left( \frac{\partial \psi}{\partial r} \right),$$

$$w = - \left( \frac{1}{r} \right) \left( \frac{\partial \psi}{\partial x} \right), \quad T - T_\infty = \Delta T \left( \frac{x}{l} \right) \theta(\eta), \quad g(\eta) = \frac{a^*}{a_0}, \quad h(\eta) = \frac{b^*}{b_0}, \tag{12}$$

the incompressibility constraint is verified trivially while expressions (2)–(6) are reduced to

$$\left. \begin{aligned} & \frac{1}{(1 - \phi)^{2.5} \left( \frac{1 - \phi + \phi \frac{\rho_s}{\rho_f}}{1 - \phi + \phi \frac{\rho_s}{\rho_f}} \right)} [(1 + 2\gamma\eta)f''' + 2\gamma f'''] + f'^2 + \beta^{*2} \\ & + \frac{M}{\left( \frac{1 - \phi + \phi \frac{\rho_s}{\rho_f}}{1 - \phi + \phi \frac{\rho_s}{\rho_f}} \right)} [\beta^* - f'] + \frac{\left( \frac{1 - \phi + \phi \frac{\rho_s}{\rho_f}}{1 - \phi + \phi \frac{\rho_s}{\rho_f}} \right)}{\left( \frac{1 - \phi + \phi \frac{\rho_s}{\rho_f}}{1 - \phi + \phi \frac{\rho_s}{\rho_f}} \right)} \lambda \theta = 0, \end{aligned} \right\} \tag{13}$$

$$\frac{\frac{k_{nf}}{k_f}}{\left( 1 - \phi + \phi \frac{(\rho C_p)_s}{(\rho C_p)_f} \right)} [(1 + 2\gamma\eta)\theta'' + 2\gamma\theta'] + \text{Pr}(f\theta' + f'\theta) = 0, \tag{14}$$

$$\frac{1}{Sc} [(1 + 2\gamma\eta)g'' + 2\gamma g'] + fg' - kgh^2 = 0, \tag{15}$$

$$\frac{\delta}{Sc} [(1 + 2\gamma\eta)h'' + 2\gamma h'] + fh' - kgh^2 = 0, \tag{16}$$

$$f = V_w, \quad f' = 0, \quad \theta = 1, \quad g' = k_s g, \quad \delta h' = -k_s g \text{ at } \eta = 0,$$

$$f' \rightarrow \beta^*, \quad \theta \rightarrow 0, \quad g \rightarrow 0, \quad h \rightarrow 0 \text{ when } \eta \rightarrow \infty. \tag{17}$$

Here  $\lambda \left( = \frac{Gr}{Re^2} \right)$  denotes the mixed convection parameter,  $Gr \left( = \frac{g\beta_f \Delta T l^3}{\nu^2} \right)$  the Grashof number,  $\gamma \left( = \frac{\gamma l}{U_\infty a^2} \right)^{0.5}$  the curvature parameter,  $V_w \left( = \frac{r}{a} \left( \frac{l}{v_f U_\infty} \right)^{0.5} V_w^* \right)$  permeability parameter,  $M \left( = \frac{\sigma B_0^2}{\rho_f \left( \frac{U_\infty}{\nu} \right)} \right)$  the magnetic parameter,  $K \left( = \frac{k_s a_0^2 l}{U_\infty} \right)$  the homogeneous parameter,  $\beta^* \left( = \frac{u_\infty}{u_0} \right)$  the velocities ratio,  $K_s \left( = \frac{k_s}{D_A} \sqrt{\frac{\gamma l}{U_\infty}} \right)$  the heteroge-

neous parameter,  $Re_x \left( = \frac{U_\infty l}{\nu} \right)$  the local Reynolds number,  $Pr \left( = \frac{\nu}{\alpha} \right)$  the Prandtl number and  $\delta \left( = \frac{D_A}{D_s} \right)$  the diffusion coefficient with ratio of mass.

Putting  $\delta = 1$  and  $g(\eta) + h(\eta) = 1$  then Eqs. (10)–(12) become

$$\frac{1}{Sc} [(1 + 2\gamma\eta)g'' + 2\gamma g'] + fg' - Kg(1 - g)^2 = 0, \tag{18}$$

$$g' = K_s g \text{ at } \eta \rightarrow 0, \quad g \rightarrow 1 \text{ at } \eta \rightarrow \infty. \tag{19}$$

Mathematical expression for surface drag force and heat transfer rate are

$$C_f = \frac{\tau_w}{\rho_f U_\infty^2}, \quad Nu_x = \frac{lq_w}{k_f \Delta T}, \tag{20}$$

where

$$\tau_w = \mu_{nf} \left| \frac{\partial u}{\partial r} \right|_{r=a},$$

$$q_w = -k_f \left( \frac{\partial T}{\partial r} \right)_{r=a}. \tag{21}$$

Invoking Eq. (21) in Eq. (20) we take the following dimensionless forms

$$Re_x^{0.5} C_{fx} = \left( \frac{\bar{x}}{(1 - \phi)^{2.5}} f''(0) \right), \quad Re_x^{-0.5} Nu_x = - \frac{k_{nf}}{k_f} \bar{x} \theta'(0), \tag{22}$$

in which  $\bar{x} = \frac{x}{l}$ .

### Discussion

The differential systems consisting of Eqs. (13), (14), (18) and (17), (19) have been solved numerically by built-in-Shooting method in mathematica. Numerical computations are carried out for several set of variables known as Prandtl number (Pr), mixed convection parameter ( $\lambda$ ), curvature parameter ( $\gamma$ ), permeability parameter ( $V_w$ ), magnetic parameter ( $M$ ), Schmidt number ( $Sc$ ), nanoparticle volume fraction ( $\phi$ ), homogeneous reaction parameter ( $k$ ) and heterogeneous reaction parameter ( $k_s$ ). For physical insights of velocity  $f'(\eta)$ , temperature  $\theta(\eta)$  and concentration  $g(\eta)$ , the Figs. 2–17 have been displayed.

Influence of curvature ( $\gamma$ ) parameter on the fluid velocity field for positive values of mixed convection ( $\lambda$ ) parameter is shown in Fig. 2. There is an enhancement of  $f'(\eta)$  for larger ( $\gamma$ ). Since for larger estimation of ( $\gamma$ ) the radius of cylinder decays which reduces the contact region of cylinder. That is why  $f'(\eta)$  enhances. Role of nanoparticle volume fraction ( $\phi$ ) on  $f'(\eta)$  is displayed in Fig. 3.  $f'(\eta)$  is noticed an increasing function of ( $\phi$ ). Fig. 4 reports the salient characteristics of mixed convection parameter ( $\lambda$ ) in Fig. 4. Here  $f'(\eta)$  enhances for larger ( $\lambda$ ). Since  $\lambda$  is the combination of buoyancy forces and viscous forces. In fact higher estimation of mixed convection ( $\lambda$ ) parameter correspond to decay in viscous forces and so an augmentation in  $f'(\eta)$  is distinguished.

**Table 1**  
Thermal characteristics of continuous phase fluid and nanomaterials [2]:

| Continuous phase fluid and nanomaterials | Water            | Aluminum oxide                 | Titanium dioxide | Copper |
|--|------------------|--------------------------------|------------------|--------|
| Molecular formula                        | H <sub>2</sub> O | Al <sub>2</sub> O <sub>3</sub> | TiO <sub>2</sub> | Cu     |
| C <sub>p</sub> (J/kg K)                  | 4179             | 765                            | 686.2            | 385    |
| ρ (kg/m <sup>3</sup> )                   | 997.1            | 3970                           | 4250             | 8933   |
| k (W/mK)                                 | 0.613            | 40.0                           | 8.954            | 400.0  |
| α × 10 <sup>7</sup> (m <sup>2</sup> /s)  | 1.47             | 131.1                          | 30.9             | 1163.1 |
| β × 10 <sup>-5</sup> (1/K)               | 21               | 0.85                           | 0.9              | 1.67   |

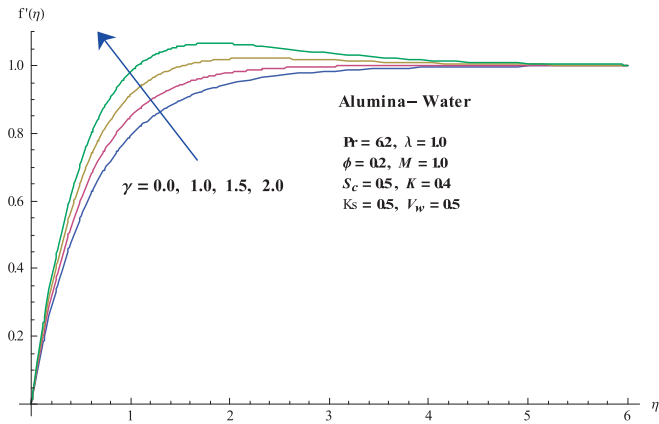


Fig. 2.  $\gamma$  via  $f'(\eta)$ .

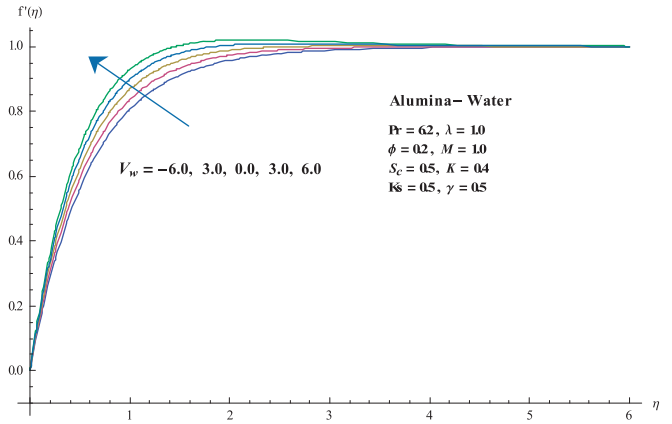


Fig. 5.  $V_w$  via  $f'(\eta)$ .

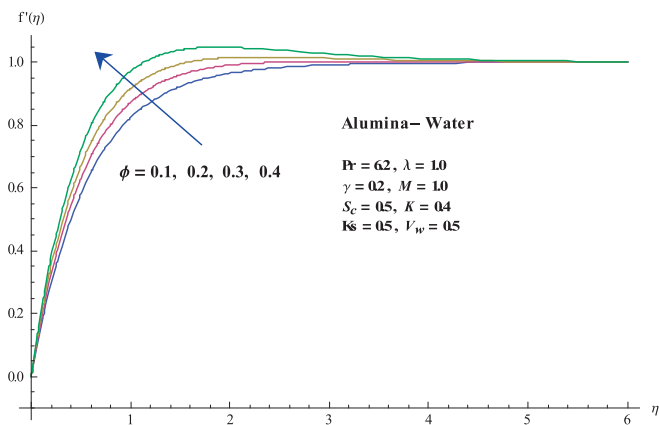


Fig. 3.  $\phi$  via  $f'(\eta)$ .

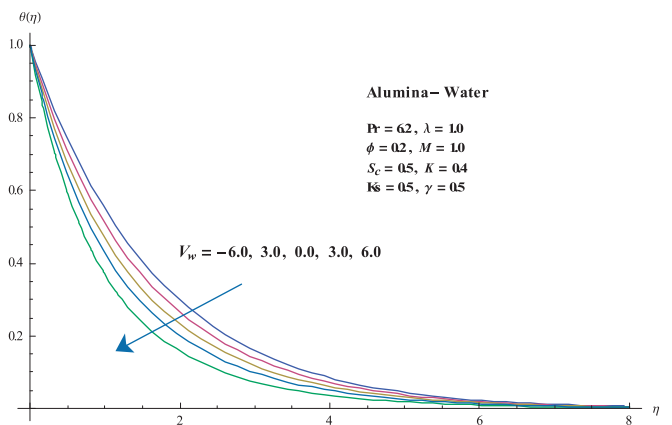


Fig. 6.  $V_w$  via  $\theta(\eta)$ .

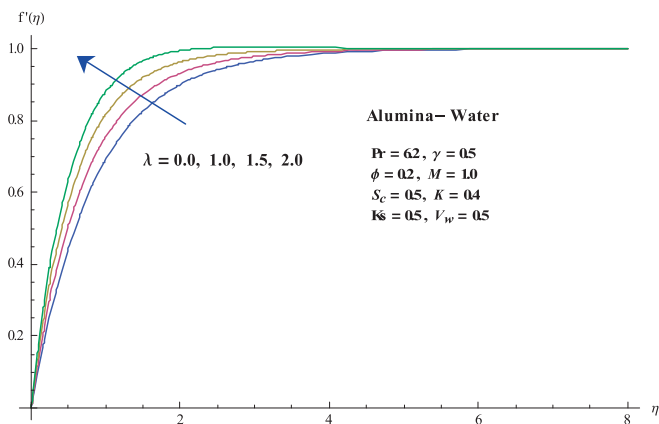


Fig. 4.  $\lambda$  via  $f'(\eta)$ .

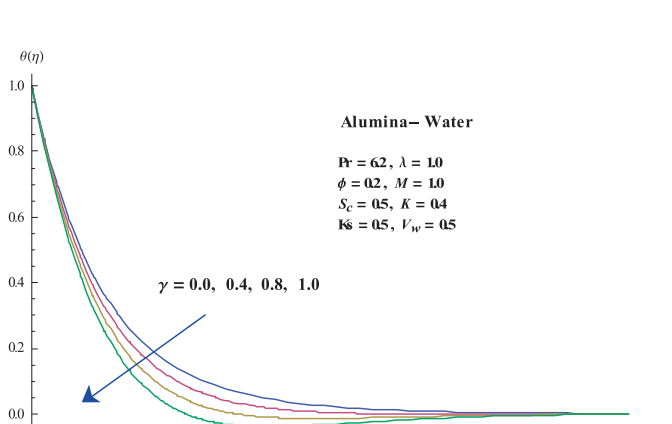


Fig. 7.  $\gamma$  via  $\theta(\eta)$ .

Characteristics of permeability parameter ( $V_w$ ) on  $f'(\eta)$  is elucidated in Fig. 5. Here velocity distribution enhances for larger ( $V_w$ ). However opposite trend is observed for temperature  $\theta(\eta)$  (see Fig. 6). Effect of curvature parameter ( $\gamma$ ) on  $\theta(\eta)$  is sketched in Fig. 7. Here  $\theta(\eta)$  decreases via ( $\gamma$ ). There is a decrease in resistance for larger ( $\gamma$ ) and so  $\theta(\eta)$  decreases. Fig. 8 demonstrates impact of nanoparticle volume fraction ( $\phi$ ) on  $\theta(\eta)$ . As expected for larger nanoparticle volume fraction ( $\phi$ ) there is an increase in thermal conductivity of fluid. As a result both  $\theta(\eta)$  and thermal layer thick-

ness are increased. Fig. 9 illustrates decay of temperature and thermal layer thickness for larger mixed convection parameter ( $\lambda$ ). Fig. 10 depicts the impact of ( $M$ ) on  $\theta(\eta)$ . For larger  $M$  there is more resistive type force which slows down the flow. Further  $\theta(\eta)$  decreases via  $M$ . Fig. 11 presents the behavior of Prandtl number on temperature field. Here temperature is a decreasing function of varying estimation of Prandtl number. Characteristics of curvature ( $\gamma$ ) on concentration  $g(\eta)$  are displayed in Fig. 12. Here concentration field shows decreasing behavior for rising values of ( $\gamma$ ).

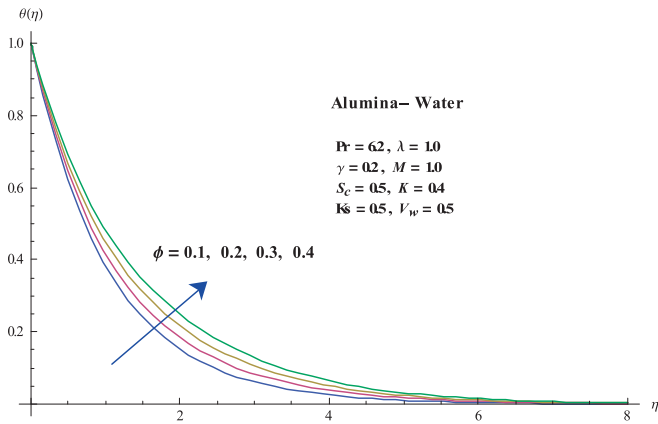


Fig. 8.  $\phi$  via  $\theta(\eta)$ .

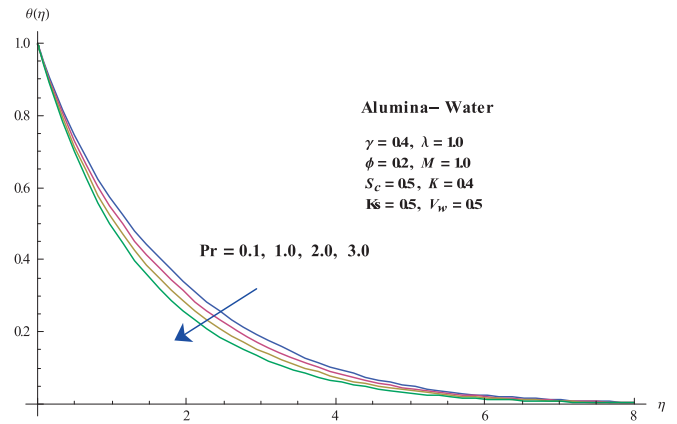


Fig. 11. Pr via  $\theta(\eta)$ .

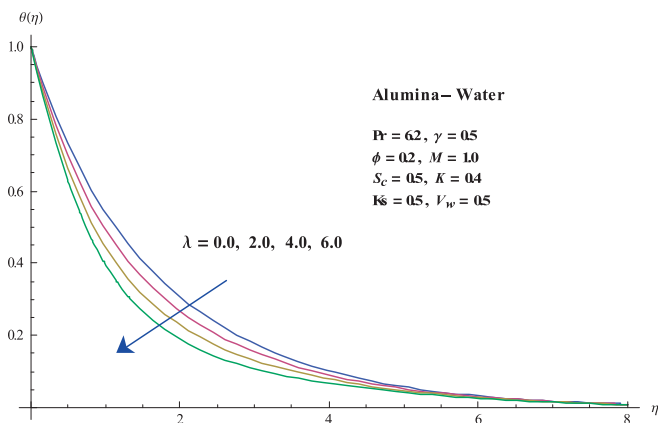


Fig. 9.  $\lambda$  via  $\theta(\eta)$ .

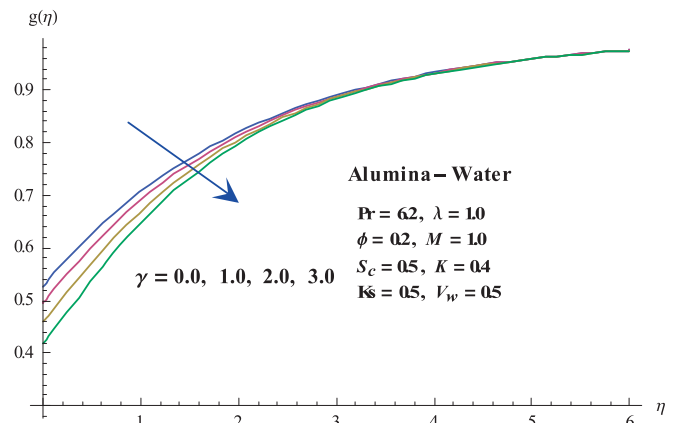


Fig. 12.  $\gamma$  via  $g(\eta)$ .

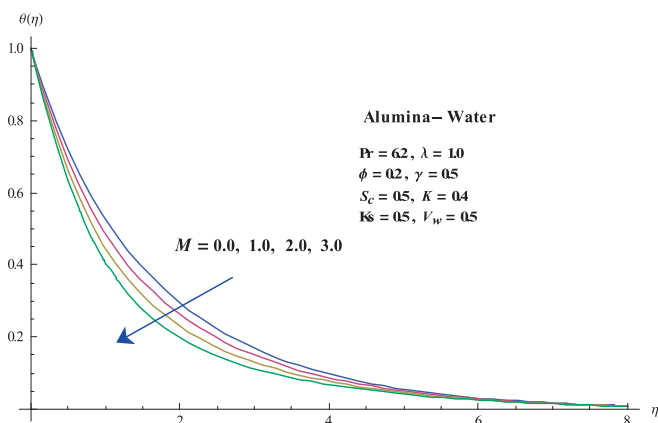


Fig. 10.  $M$  via  $\theta(\eta)$ .

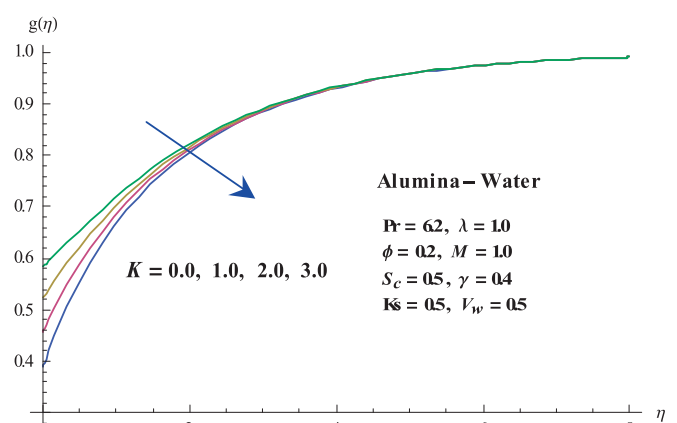


Fig. 13.  $K$  via  $g(\eta)$ .

Influence of homogeneous reaction parameter ( $K$ ) on  $g(\eta)$  is sketched in Fig. 13. Concentration  $g(\eta)$  decays while associated layer thickness enhances for larger ( $K$ ). Behavior of heterogeneous reaction parameter ( $Ks$ ) on  $g(\eta)$  is analyzed in Fig. 14. Here  $g(\eta)$  enhances for larger variations of heterogeneous reaction parameter ( $Ks$ ). Fig. 15 elucidates the variation of ( $Sc$ ) on  $g(\eta)$ . As ( $Sc$ ) is inversely proportional to coefficient of Brownian diffusion. Higher ( $Sc$ ) corresponds to weaker Brownian diffusion. It give rise to decay in  $g(\eta)$ . Figs. 16 and 17 correspond to results of ( $\gamma$ ) and ( $M$ ) on surface drag force and heat transfer rate. It is worth mentioning that both graphs in Figs. 16 and 17 have been plotted for copper-water nano-

material. It is observed that surface drag force and heat transfer rate are enhanced for larger ( $\gamma$ ) and ( $M$ ).

**Conclusions**

Following points are the observations of presented study.

- $f'(\eta)$  enhances for higher  $\gamma$ ,  $\phi$  and  $\lambda$ .

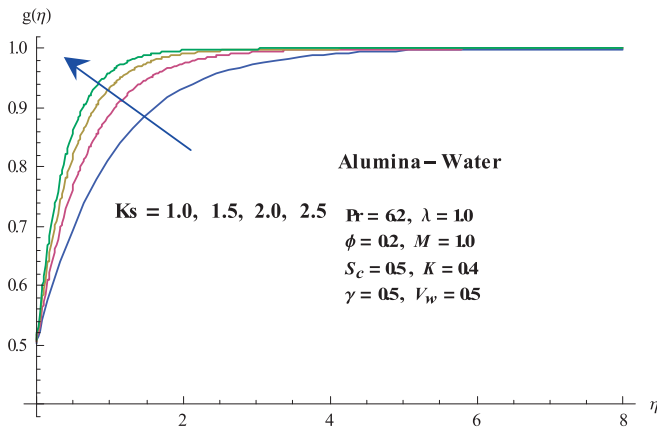


Fig. 14.  $K_s$  via  $g(\eta)$ .

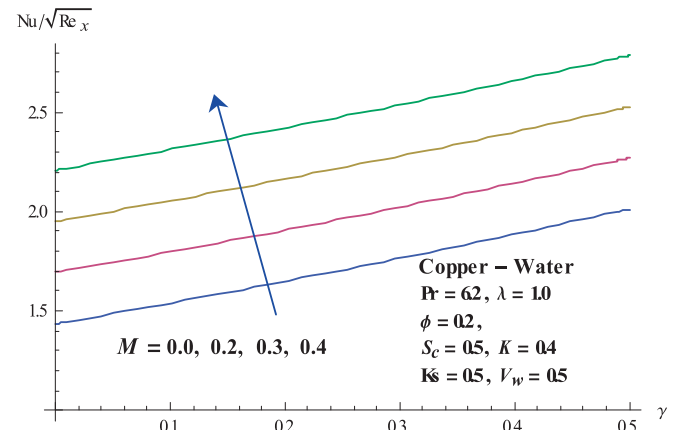


Fig. 17. Effects of  $\gamma$  and  $M$  on  $Nu_x$ .

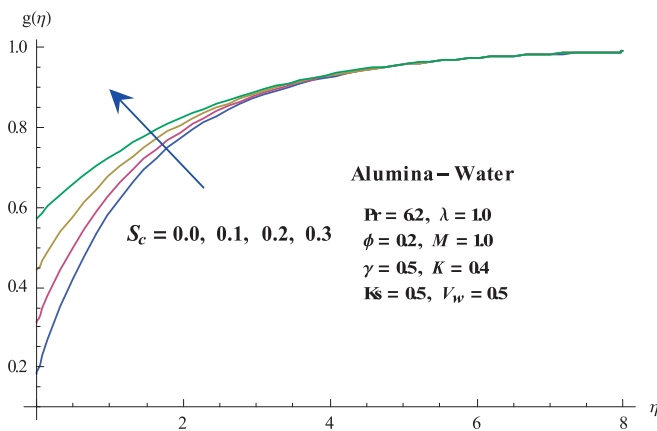


Fig. 15.  $S_c$  via  $g(\eta)$ .

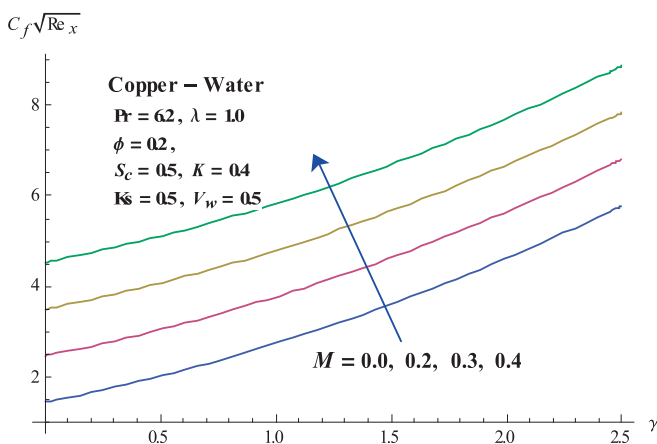


Fig. 16. Effects of  $\gamma$  and  $M$  on  $C_{f_x}$ .

- Larger nanoparticles volume fraction ( $\phi$ ) rises  $\theta(\eta)$  and thermal layer thickness.
- An increase in curvature ( $\gamma$ ) and homogeneous reaction ( $K$ ) parameters lead to reduce concentration  $g(\eta)$ .
- Thermal layer thickness is decreased for  $M$  and  $Pr$ .
- Behavior of  $Re_x^{0.5} C_{f_x}$  for larger ( $\gamma$ ) and ( $M$ ) is increasing.
- $Re_x^{-0.5} Nu_x$  enhances for larger ( $\gamma$ ) and ( $M$ ).

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