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Nurul Aini Jaafar; Yazariah Mohd Yatim; D. S. Sankar



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Mathematical Analysis For Unsteady Dispersion of Solute With Chemical Reaction In Blood Flow

Nurul Aini Jaafar^{1, a)}, Yazariah Mohd Yatim^{1, b)} and D. S. Sankar^{2, c)}

¹*School of Mathematical Sciences, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia*

²*Engg. Mathematics Unit, Faculty of Engg., Universiti Teknologi Brunei, Gagong, BE1410, Brunei Darussalam*

^{a)}Corresponding author: nurulaini_math@yahoo.com

^{b)}yazariahmy@usm.my

^{c)}sankar_ds@yahoo.co.in

Abstract. The effect of chemical reaction on the unsteady dispersion of solute in blood flow through a pipe and a channel between two parallel plates is analyzed mathematically, treating the blood as Casson fluid. Generalized dispersion model is applied to solve the convective-diffusion equation. It is seen that the dispersion function at steady state and relative axial diffusivity decrease with the increase of chemical reaction rate while the reverse behavior is shown by dispersion function at unsteady state. The dispersion function increases with the increase of yield stress at the center. The dispersion function is considerably higher when the solute disperses in channel flow than in pipe flow and the reverse behavior is depicted by the relative axial diffusivity.

Keywords: Unsteady dispersion of solute; Chemical reaction; Blood flow; Casson fluid model; Effective axial diffusivity

PACS: 47.85.-g

INTRODUCTION

The study of solute dispersion in fluid flow is essential for dealing the important physical phenomenon in biophysics, physiological fluid dynamics, biomechanics, bio-medical engineering etc. Some specific applications are the mixing and transport of drugs in physiological systems, dispersion of gaseous tracer in chemical engineering, transport of pollutants in the environment engineering etc. [1-3]. Taylor [4] was the pioneer who investigated the basic theory of solute dispersion in pipe by dealing with the experiments. He reported that the solute disperses in the solvent due to the combined action of molecular diffusion and non-uniform velocity distribution. He found the effective axial diffusivity in tube as $\bar{D}_{eff} = \bar{a}^2 \bar{u}_m^2 / 48 \bar{D}_m$, where \bar{a} is the pipe radius, \bar{u}_m is the mean velocity and \bar{D}_m is the molecular diffusivity. Aris [5] stated that the Taylor's theory is valid only when $\bar{D}_{eff} \gg \bar{D}_m$. He then extended Taylor's theory as $\bar{D}_{eff} = \bar{D}_m + \bar{a}^2 \bar{u}_m^2 / 48 \bar{D}_m$ by including the effect of axial molecular diffusivity \bar{D}_m .

Bailey and Gogarty [6] studied the unsteady dispersion of solute by ignoring the axial diffusion using the finite difference method. Ananthakrishnan et al. [7] studied the solute dispersion by considering both radial and axial diffusions using finite difference method. They propounded that the Taylor-Aris's theory gives a good description if the time after injection of the solute exceeds $0.5(\bar{a}^2 / \bar{D}_m)$. However, normally the dispersion in cardiovascular system is small. Gill [8] proposed a series expansion for solving the convective-diffusion equation and his solution tends to be more general for all time. Gill and Sankarasubramanian [9] extended the theory to the generalized dispersion model (GDM) and obtained a series solution which described the whole dispersion process.

The study of solute dispersion for steady dispersion in non-Newtonian fluids such as Casson, power-law and Bingham fluids through pipe and channel was analyzed by Sharp [10] using Taylor-Aris's theory. Dash et al. [11] investigated the unsteady dispersion of solute in Casson fluid through pipe and channel using GDM. The solute dispersion of nanoparticles within the tumor in blood vessels with permeable wall has been studied by many

researchers [12-15]. Sankar et al. [16] and Jaafar et al. [17] analyzed the steady dispersion of solute in blood flow through pipe and channel for Herschel-Bulkley fluid using the approach of Taylor-Aris and GDM, respectively.

In the studies mentioned so far, it is assumed that the solute does not chemically react with fluid. Bird et al. [18] reported that in a wide variety of chemical engineering problems, the diffusion of solute takes place simultaneously with chemical reaction. The unsteady dispersion of solute in Newtonian and non-Newtonian fluids in the presence of chemical reaction in a pipe and a channel using Taylor's theory has been studied by many researchers [19-22]. To the authors' knowledge, the study of unsteady dispersion of solute with chemical reaction using GDM in Casson fluid has not been carried out. Hence, the present study examines the unsteady dispersion of solute in Casson fluid through a pipe and a channel in the presence of chemical reaction using GDM.

MATHEMATICAL FORMULATION

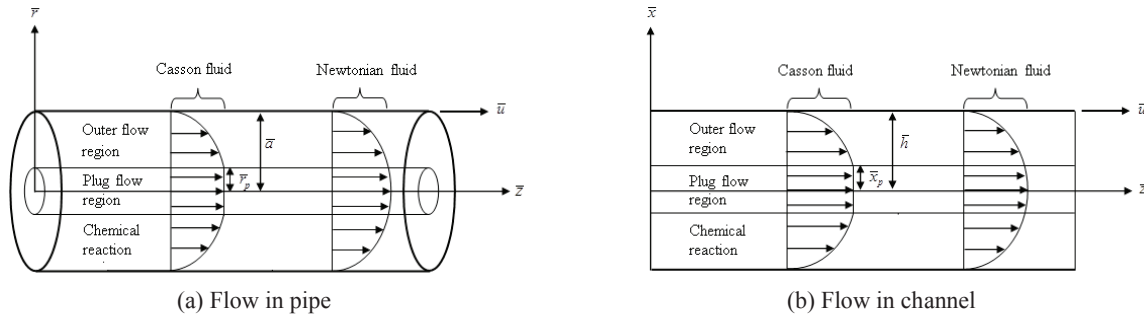


FIGURE 1. The geometries of fluid flow.

Consider the laminar, steady, axi-symmetric and fully-developed unidirectional flow of blood (assumed as viscous incompressible fluid) in a straight pipe and a channel, treating blood as Casson fluid. The geometries of fluid flowing in a pipe and a channel are depicted in Figs. 1(a) and (b), respectively, where \bar{u} is the axial velocity of fluid, \bar{r} , \bar{x} and \bar{z} are the coordinates in the radial, transverse and axial directions, respectively, \bar{r}_p and \bar{x}_p are the plug flow radius and semi-width, respectively and \bar{a} and \bar{h} are the radius of pipe and semi-width of channel, respectively.

Flow in Pipe

Governing equations

Consider the unsteady dispersion of solute in pipe flow with initial length \bar{z}_s units. The cylindrical polar coordinate system $(\bar{r}, \bar{\psi}, \bar{z})$ is used where $\bar{\psi}$ is the azimuthal angle. The axial components of momentum equations where the velocities in $\bar{\psi}$ and \bar{z} direction are assumed negligible small which satisfies Navier-Stokes equation as

$$\frac{d\bar{p}}{d\bar{z}} = -\frac{1}{\bar{r}} \frac{d}{d\bar{r}} (\bar{r}\bar{\tau}), \quad (1)$$

$$\frac{d\bar{p}}{d\bar{r}} = 0, \quad (2)$$

where \bar{p} is the pressure and $\bar{\tau}$ is the shear stress. Eqs. (1) and (2) show that the pressure varies only in the axial direction and constant in the radial direction. The constitutive equations of Casson fluid model are as follows:

$$-\frac{d\bar{u}}{d\bar{r}} = \begin{cases} \frac{1}{\bar{\mu}} (\sqrt{\bar{\tau}} - \sqrt{\bar{\tau}_y})^2 & \text{if } \bar{\tau} > \bar{\tau}_y \\ 0 & \text{if } \bar{\tau} \leq \bar{\tau}_y \end{cases}, \quad (3)$$

where $\bar{\tau}_y$ is the yield stress and $\bar{\mu}$ is the viscosity of Casson fluid. Eq. (3) indicates that the normal shear flow (outer flow) occurs when $\bar{\tau} > \bar{\tau}_y$ and the unshear flow (solid-like flow or plug flow) occurs when $\bar{\tau} \leq \bar{\tau}_y$. The boundary conditions are given by:

$$\bar{\tau} \text{ finite at } \bar{r} = 0 \text{ and } \bar{u} = 0 \text{ at } \bar{r} = \bar{a}. \quad (4)$$

The unsteady convective-diffusion equation with chemical reaction in a pipe flow is given by

$$\frac{\partial \bar{C}}{\partial \bar{t}} + \bar{u} \frac{\partial \bar{C}}{\partial \bar{z}} = \bar{D}_m \left\{ \frac{1}{\bar{r}} \frac{\partial}{\partial \bar{r}} \left(\bar{r} \frac{\partial \bar{C}}{\partial \bar{r}} \right) + \frac{\partial^2 \bar{C}}{\partial \bar{z}^2} \right\} - \bar{R} \bar{C}, \quad (5)$$

where $\bar{C}(\bar{r}, \bar{z}, \bar{t})$ is the concentration of solute, \bar{t} is the time variable, \bar{R} is the rate of chemical reaction. The initial and boundary conditions of solute concentration $\bar{C}(\bar{r}, \bar{z}, \bar{t})$ with reference concentration \bar{C}_0 are as follows:

$$\bar{C}(\bar{r}, \bar{z}, 0) = \begin{cases} \bar{C}_0 & \text{if } |\bar{z}| \leq \bar{z}_s/2, \\ 0 & \text{if } |\bar{z}| > \bar{z}_s/2, \end{cases} \quad (6)$$

$$\bar{C}(\bar{r}, \infty, \bar{t}) = 0, \quad (7)$$

$$\frac{\partial \bar{C}}{\partial \bar{r}}(0, \bar{z}, \bar{t}) = 0 = \frac{\partial \bar{C}}{\partial \bar{r}}(\bar{a}, \bar{z}, \bar{t}), \quad (8)$$

Non-dimensional variables

Let us introduce the following non-dimensional variables:

$$C = \frac{\bar{C}}{\bar{C}_0}, u = \frac{\bar{u}}{\bar{u}_0}, r = \frac{\bar{r}}{\bar{a}}, r_p = \frac{\bar{r}_p}{\bar{a}}, z = \frac{\bar{D}_m \bar{z}}{\bar{a}^2 \bar{u}_0}, t = \frac{\bar{D}_m \bar{t}}{\bar{a}^2}, \tau = \frac{\bar{t}}{\bar{\mu} \bar{u}_0 / \bar{a}}, \tau_y = \frac{\bar{\tau}_y}{\bar{\mu} \bar{u}_0 / \bar{a}}, \alpha = \sqrt{\frac{\bar{a}^2 \bar{R}}{\bar{D}_m}}, Pe = \frac{\bar{a} \bar{u}_0}{\bar{D}_m}, \quad (9)$$

where \bar{u}_0 is the characteristic velocity given by [11], α is the chemical reaction rate and Pe is the Péclet number.

Solution method

Using Eq. (9) in Eqs. (1)-(8), we get the corresponding equations in non-dimensional forms as

$$\frac{dp}{dz} = -\frac{1}{r} \frac{d}{dr} (r\tau), \quad (10)$$

$$\frac{dp}{dr} = 0, \quad (11)$$

$$-\frac{du}{dr} = \begin{cases} (\sqrt{\tau} - \sqrt{\tau_y})^2 & \text{if } \tau > \tau_y, \\ 0 & \text{if } \tau \leq \tau_y, \end{cases} \quad (12)$$

$$\tau \text{ finite at } r = 0 \text{ and } u = 0 \text{ at } r = 1, \quad (13)$$

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial z} = \left\{ \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C}{\partial r} \right) + \frac{1}{Pe^2} \frac{\partial^2 C}{\partial z^2} \right\} - \alpha^2 C, \quad (14)$$

$$C(r, z, 0) = \begin{cases} 1 & \text{if } |z| \leq z_s/2, \\ 0 & \text{if } |z| > z_s/2, \end{cases} \quad (15)$$

$$C(r, \infty, t) = 0, \quad (16)$$

$$\frac{\partial C}{\partial r}(0, z, t) = 0 = \frac{\partial C}{\partial r}(1, z, t). \quad (17)$$

Eq. (10) yields $\tau = -(r/2)/(dp/dz)$ and substituting $\tau = -(r/2)/(dp/dz)$ into (12) and integrating Eq. (12) with respect to r yields the velocity in the outer and plug flow regions as given by [11] in Eq. (11a) and (11b), respectively. The solution of $C(r, z, t)$ is first assumed using the approach of [9] as follows:

$$C(r, z, t) = C_m(z_1, t) + \sum_{j=1}^{\infty} f_j(r, t) \frac{\partial^j C_m(z_1, t)}{\partial z_1^j}, \quad (18)$$

where $C_m = 2 \int_0^1 Cr dr$ is the mean concentration, $f_j(r, t)$ is the dispersion function and $z_1 = z - u_m t$ is a new axial coordinate, where u_m is non-dimensional of mean velocity given by [11] in Eq. (13). Following [9], multiplying Eq. (14) by $2r$ and substituting mean concentration yields GDM as

$$\frac{\partial C_m}{\partial t} = \sum_{j=1}^{\infty} K_j(t) \frac{\partial^j C_m}{\partial z_1^j} - \alpha^2 C_m, \quad (19)$$

where $K_j(t)$ is the dispersion coefficient. Substituting Eq. (18) into Eq. (14) and using Eq. (19) yields the series expansion. The function of f_1 in Eq. (18) is the most essential to measure C . Equating the coefficients of $\partial^j C_m / \partial z_1^j$ and let $f_1(r, t) = f_{1s}(r) + f_{1t}(r, t)$, where f_{1s} is the steady state and f_{1t} is the unsteady state. Solving f_1 numerically using *Mathematica* program (DSolve) subject to the conditions $f_j(r, 0) = 0$, $(df_j/dr)(0, t) = 0 = (df_j/dr)(1, t)$ for $j = 1, 2, \dots$, let the steady dispersion function in the plug flow region as $f_{1s}(r)$ and it is given by

$$f_{1s-}(r) = -\frac{1}{\alpha^2} \left[\frac{1}{2} - \frac{32}{21} r^{\frac{1}{2}} + \frac{4}{3} r_p - \frac{r_p^2}{3} + \frac{r_p^4}{42} \right] + CI_1 J_0(i\alpha r) \text{ if } 0 \leq r \leq r_p, \quad (20)$$

where J_0 is the Bessel's functions of first kind of order zero and CI_1 is a constant. The steady dispersion function in the outer flow region, $f_{1s+}(r)$ if $r_p \leq r \leq 1$ is not shown in this paper because of long expression. CI_1 is computed by Simpson rule 3/8 using the solvability condition $\int_0^1 f_j r dr = 0$ which is formed by substituting Eq. (18) into mean concentration. The solution of $f_{1t}(r, t)$ as follows:

$$f_{1t}(r, t) = e^{-\alpha^2 t} \sum_{m=1}^{\infty} A_m e^{-\lambda_m^2 t} J_0(\lambda_m r), \quad (21)$$

where λ_m is the root of $J_1(\lambda_m) = 0$ from $f_j(r, 0) = 0$, J_1 is the Bessel's functions of first kind of order one and $A_m = -\frac{2}{J_0^2(\lambda_m) + J_1^2(\lambda_m)} \left(\int_0^{r_p} r J_0(\lambda_m r) f_{1s-} dr + \int_{r_p}^1 r J_0(\lambda_m r) f_{1s+} dr \right)$ is computed numerically by Simpson's rule 3/8.

Flow in Channel

Governing equations

Cartesian coordinate is used to describe the solute dispersion in a channel flow. The momentum and unsteady convective-diffusion equations with chemical reaction in a channel flow are as follows:

$$\frac{d\bar{p}}{dz} = -\frac{d\bar{\tau}}{dx}, \quad (22)$$

$$\frac{d\bar{p}}{dx} = 0, \quad (23)$$

$$\frac{\partial \bar{C}}{\partial t} + \bar{u} \frac{\partial \bar{C}}{\partial z} = \bar{D}_m \left\{ \frac{\partial^2 \bar{C}}{\partial x^2} + \frac{\partial^2 \bar{C}}{\partial z^2} \right\} - \bar{R} \bar{C}. \quad (24)$$

Solution method

The velocity of Casson fluid in the outer and plug flow regions are gained via same approach given by [11] in Eqs. (45a) and (45b), respectively. The solution of convective-diffusion equation is assumed as in Eq. (18) in terms of x replacing r for Cartesian coordinate, where $C_m = \int_0^1 C dx$. Using similar boundary conditions as in pipe flow in terms of x , the dispersion function at steady state in the plug flow region, $f_{1s-}(x)$ is given by

$$f_{1s-}(x) = -\frac{1}{\alpha^2} \left[\frac{1}{3} - \frac{16}{15} x^{\frac{1}{2}} + x_p - \frac{x_p^2}{3} + \frac{x_p^3}{15} \right] + CI_2 (e^{-\alpha x} + e^{\alpha x}) \text{ if } 0 \leq x \leq x_p, \quad (25)$$

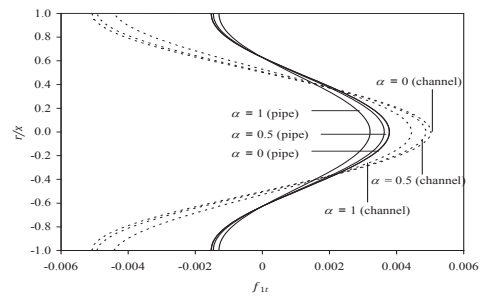
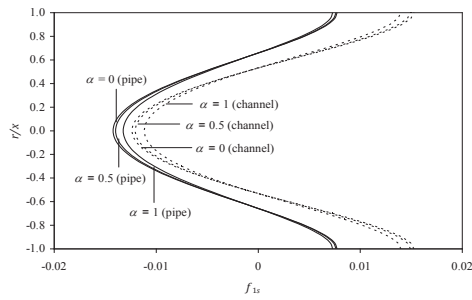
where $f_{1s+}(x)$ if $x_p \leq x \leq 1$ is not shown because of long expression and constant CI_2 is computed numerically by Simpson's rule 3/8. The following expressions for unsteady state dispersion function through the channel as follows:

$$f_{1t}(x, t) = e^{-\alpha^2 t} \sum_{m=1}^{\infty} A_m e^{-\lambda_m^2 t} \cos(\lambda_m x), \quad (26)$$

where $A_m = -2 \left(\int_0^{x_p} \cos(\sqrt{\lambda_m^2 - \alpha^2} x) f_{1s-} dx + \int_{x_p}^1 \cos(\sqrt{\lambda_m^2 - \alpha^2} x) f_{1s+} dx \right)$ is computed numerically using Simpson's rule 3/8.

RESULTS AND DISCUSSIONS

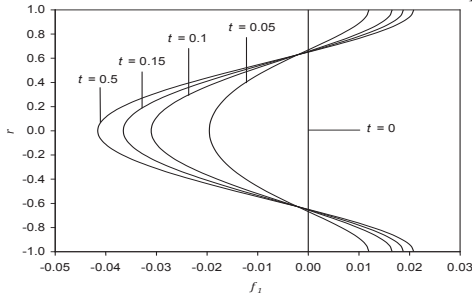
Figures 2(a) and (b) exhibit the variation of dispersion function for steady and unsteady, respectively with r and x for different values of chemical reaction rate α at $r_p = x_p = 0.1$ in a pipe and a channel. The results are significant to measure the concentration C . Figures 2(a) and (b) illustrate that f_{1s} increases, while, f_{1t} decreases considerably with the increase of r/x , respectively. It is noted that f_{1s} increases, while, f_{1t} decreases when α increases at the center. It is observed that f_{1s} and f_{1t} are higher when the solute disperses in a channel than in a pipe at the center. When substituting $\alpha = 0$ into $f_{1s-}(r)$, $f_{1s+}(r)$ and $f_{1t}(r, t)$, the results show the dispersion function without chemical reaction and in a good agreement with [11] in Eqs. (32a), (32b) and (34), respectively. Then, the results of $f_{1s-}(x)$, $f_{1s+}(x)$ and $f_{1t}(r, t)$ show in a good agreement with [11] in Eqs. (49a), (49b) and (51) when $\alpha = 0$, respectively.



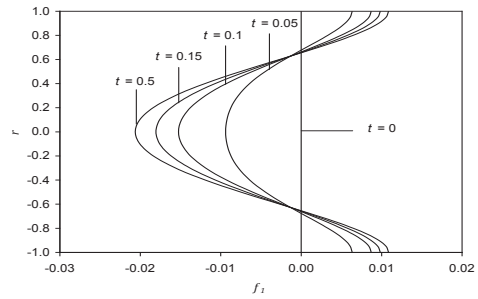
(a) Steady dispersion function

(b) Unsteady dispersion function

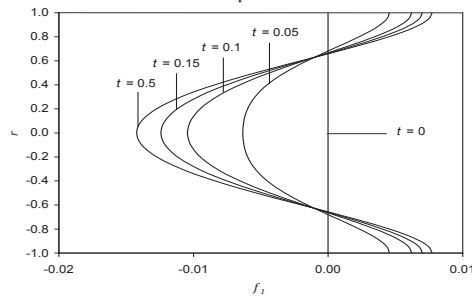
FIGURE 2. Variation of dispersion function with r and x for different values of chemical reaction rate α at $r_p = x_p = 0.1$ in a pipe and a channel.



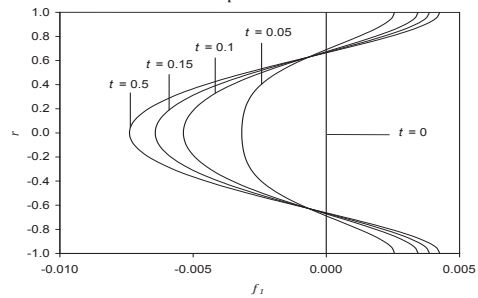
(a) $r_p = 0$



(b) $r_p = 0.05$

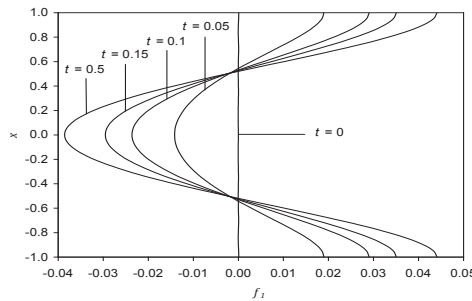


(c) $r_p = 0.1$

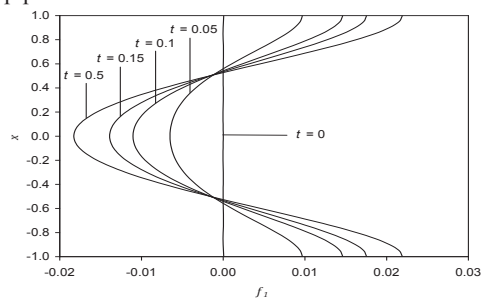


(d) $r_p = 0.2$

FIGURE 3. Variation of dispersion function f_1 with radial distance r for different values of time t and yield stress r_p at $\alpha = 0.1$ for flow in a pipe.



(a) $x_p = 0$



(b) $x_p = 0.05$

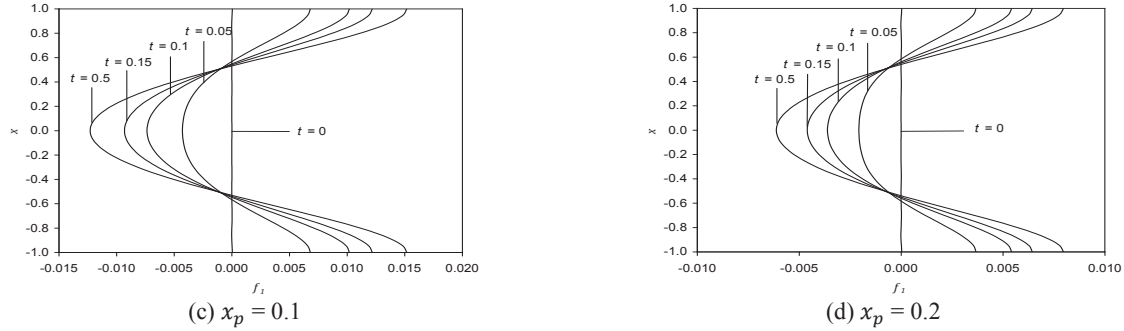


FIGURE 4. Variation of dispersion function f_1 with transverse distance x for different values of time t and yield stress x_p at chemical reaction rate $\alpha = 0.1$ for flow in a channel.

Figures 3(a)-(d) show the variation of dispersion function f_1 with radial distance r for different values of time t and yield stress $r_p = 0, 0.05, 0.1$ and 0.2 at chemical reaction rate $\alpha = 0.1$ for flow in a pipe. It is clear that f_1 decreases when r_p and t increase in the range of $-0.65 \leq r \leq 0.65$ and it increases in the rest of range because f_1 is independent of t at the center. It is noted that when $r_p = 0$, the dispersion function reduced to Newtonian fluid.

Figures 4(a)-(d) exhibit the variation of dispersion function f_1 with transverse distance x for different values of time t and yield stress $x_p = 0, 0.05, 0.1$ and 0.2 at chemical reaction rate $\alpha = 0.1$ for flow in a channel. f_1 decreases when t and x_p increase in the range of $-0.5 \leq x \leq 0.5$ and it increases in the rest of range. Similarly, the dispersion function reduced to Newtonian fluid when $x_p = 0$. Figures 3 and 4 depict that f_1 is higher when the solute disperses in a channel flow than pipe flow. It is seen that Figs. 3 and 4 decreases with the increase of α when compared to Figs. 4 and 5 in [11], respectively and when $\alpha = 0$, the dispersion function f_1 shows in a good agreement with [11].

Figures 5(a) and (b) depict the variation of relative axial diffusivity with time t for different values of yield stress r_p at chemical rate $\alpha = 0.1$ for flow in a pipe and a channel, respectively. The relative axial diffusivity decreases when the yield stress and α increases for both cases of pipe and channel when compared to Fig. 3 in [11]. It is found that the relative axial diffusivity higher when the solute disperses in pipe compared to the channel and show a good agreement with [11] when $\alpha = 0$.

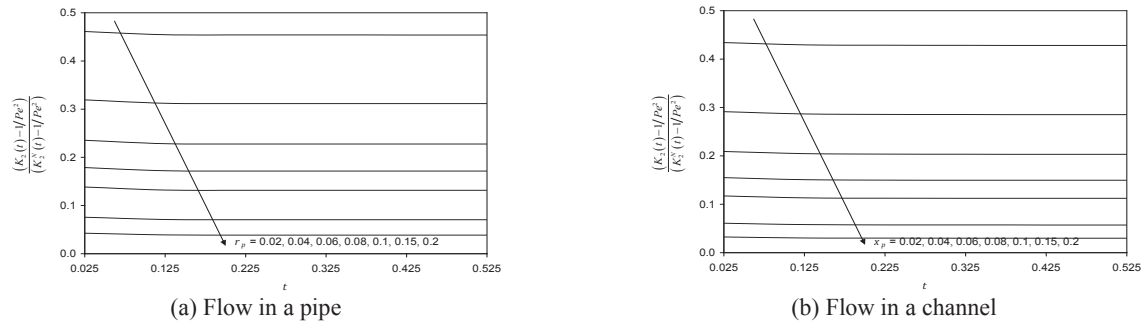


FIGURE 5. Variation of relative axial diffusivity with time t for different values of yield stress r_p and x_p at chemical reaction rate $\alpha = 0.1$.

CONCLUSIONS

The main outcomes of this analysis are summarized as follows: For flow in pipe/channel, the dispersion function and relative axial diffusivity decrease considerably with the increase of yield stress and chemical reaction rate. The dispersion function is considerably higher when the solute disperses in channel than pipe, while, the relative axial diffusivity behaves oppositely. The results obtained in this work are validated with the results of others.

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