

# Transport of Reactive Species in Oscillatory Annular Flow

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## ABSTRACT

The present article purposes to investigate the solute dispersion through an annular pipe in the presence of heterogeneous chemical reactions among the species and wall of the annulus. The solute is considered to experience a kinetic reversible phase exchange with the inner wall layer and irreversible absorption into the wall. Two kinds of oscillatory flow (Poiseuille and Couette flow) are considered in order to track the complex interactions between the velocity distributions and the reaction parameters. The method of moments as proposed by Aris-Barton is used to determine the apparent dispersion coefficient. The moment equations has been solved by using a standard finite difference implicit scheme, valid for small as well as large times. Dispersion coefficient due to the combined effect of reversible and irreversible reactions has been discussed in a variety of flow situations. Dispersion coefficient may be enhanced owing to the reversible and irreversible heterogeneous reactions in the boundary. On the basis of flow characteristics, radius ratio provides a mixed behaviour of the dispersion coefficient. Dimensionless mass proves to be an increasing function of reversible and irreversible boundary reaction parameters.

**Keywords:** Dispersion coefficient; Reversible reaction; Irreversible reaction; Phase exchange; Damköhler number.

## NOMENCLATURE

$D$	molecular diffusivity	$\nu_3$	kurtosis
$D_c$	apparent dispersion coefficient	$z$	axial coordinate
$Da$	Damköhler number	$\nu$	kinematic viscosity
$i$	time index during navigation		
$j$	space index	$\alpha_p$	frequency of pressure pulsation
$P$	Poiseuille number	$\alpha_w$	frequency of wall oscillation
$Pe$	Peclet number	$\Gamma$	irreversible reaction rate constant
$Q$	mobile phase concentration	$\delta$	Dirac delta function
$Q_s$	immobile phase concentration	$\epsilon_p$	amplitude of pressure pulsation
$r$	radial coordinate	$\epsilon_w$	amplitude of wall oscillation
$r_i$	internal radius	$\mu_q$	q-th order central moment
$r_o$	external radius	$\Omega$	phase exchange rate
$Sc$	Schmidt number	$\rho$	density
$t$	time	$\eta$	aspect ratio
$u$	axial velocity		
$\nu_2$	skewness		

## 1. INTRODUCTION

In solute transport processes, the dispersion is one of the mechanisms which is used to understand the transport of substances in a flowing stream.

Because of its extensive applications in various filed of science and technology, the study of longitudinal dispersion of tracer is of considerable interest to the scientific community. Transport in presence of wall reactions is getting more attention

since it is essential to numerous industrial and physiological circumstances, e.g., chromatography, electrophoresis, human arteries, flow through fractures etc. The behaviour of the dispersion coefficient is significantly influenced by the pulsatile nature of stream, particularly, when mean pressure gradient is smaller than the amplitude of the pulsating pressure gradient.

Taylor (1953) was the pioneer who carried out the first fundamental study on dispersion revealing the fact that, rate of broadening of species is due to the joint interactions among radial diffusion and velocity shear in the axial direction. Aris (1956) considered longitudinal diffusion for extension of Taylor's theory and developed the celebrated 'method of moments' to examine the response of the statistical variance for large times. Barton (1983) then detect certain errors in Aris's method of moments and established a new approach known as Aris-Barton method of moments which is true for all time.

The study on solute dispersion in a time-dependent Poiseuille and Couette flows have been covered by assuming pressure gradient fluctuation that can alter the flow (Aris (1960); Mazumder and Das (1992); Sarkar and Jayaraman (2004)), whereas some have made the periodic movement of the boundary wall responsible for the flow (Bandyopadhyay and Mazumder (1999), Paul (2011)). Using self-developed derivative expansion method, Sankarasubramanian and Gill (1973) studied the dispersion of solute under catalytic wall reaction. In a pulsatile flow through annulus, the consequences of wall absorption on dispersion has been discussed by Sarkar and Jayaraman (2004); Mazumder and Mondal (2005). Further more, they have highlighted the application to their model in catheterized artery. A solution of convection-diffusion equation in a two immiscible viscous fluid flowing between two parallel plates under chemical reaction has been derived analytically by Kumar, Umavathi and Basavaraj (2012). Utilizing a singular perturbation technique, the solute transport (reactive) via Newtonian fluid flowing across a thin or a long curved pipe has been studied by Marušić-Paloka and Pažanin (2011). In a subsequent work of Pažanin (2013) also discussed the same under the consideration of a Micropolar fluid flowing through a circular pipe. In solute diffusion, Mikelić, Devigne and van Duijn (2006) investigated the dispersion in a model flow through a semi-infinite two-dimensional channel, for large Peclet and Damköhler numbers. Rosencrans (1997) worked on Taylor dispersion in a curved channel and proposed that the effective diffusion can be minimized by the consideration of curvature effects. Also, if we assume a straight channel boundary, it will increase the value of effective diffusion. By extending homogenization technique, Wu and Chen (2014) studied the transverse variation of concentration for the scalar transport along a straight pipe. In a recent work of Wu, Fu and Wang, (2016), the configuration of the comprehensive spatial concentration distribution has been appropriately considered and it is reported

that instead of the flat cross-sections, solute concentration develops uniformly dispersed across a family of fixed curved transverse surfaces. However these articles were commonly restricted only with first-order irreversible reactions. Using homogenization technique, Ng and Bai (2005) studied the transport of a reactive material under the presence of reversible sorptive phase exchange at the boundary of parallel plates where the flow pulsation occurred due to movement of upper plate. Studies exist in the literature where irreversible and reversible boundary reactions are considered while discussing the dispersion process (Ng (2006); Ng and Rudraiah, (2008)).

More specifically, the present article considers the effect of pipe's annularity and flow pulsation to explore the mechanism of dispersion by the combined impact due to kinetic reversible phase exchange as well as irreversible heterogeneous reactions between the species and inner wall. The prime scope of the present work is to make a comparative study between various kinds of reactions and flows which are of great importance in the spreading of tracers in environmental and biological processes.

## 2. THE PROBLEM UNDER CONSIDERATION

An incompressible viscous fluid is supposed to flow through an annular pipe having radii denoted as  $\bar{a}$  and  $\bar{b}$  ( $\bar{a} > \bar{b}$ ), where the flow is considered unsteady, fully developed, laminar and axisymmetric. The geometry of the annulus is fixed by its radius ratio  $\eta \left( = \frac{\bar{b}}{\bar{a}} \right)$  whereas its hydraulic diameter  $d = 2(\bar{a} - \bar{b})$  determines the region of flow. Using a cylindrical coordinate system, the geometry of the annulus as depicted in Fig. 1, which indicates that radial and axial coordinates are represented by  $\bar{r}$  and  $\bar{z}$  respectively. The bars over each quantities meaning that they are dimensional.

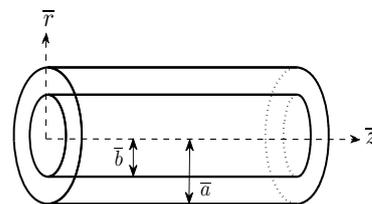


Fig. 1. Schematic diagram of the setup under consideration.

In this investigation the aspect ratio is infinite because of the infinite axial extent of the system which is also a main reason for longitudinal dispersion. Thus the independence of velocity,  $\bar{u}$ , of  $\bar{z}$  and  $\bar{\theta}$  is confirmed.

Following Schlichting (1979), the momentum equation which satisfies the velocity distribution in the longitudinal direction is,

$$\frac{\partial \bar{u}}{\partial \bar{t}} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial \bar{z}} + \nu \frac{1}{\bar{r}} \frac{\partial}{\partial \bar{r}} \left( \bar{r} \frac{\partial \bar{u}}{\partial \bar{r}} \right) \quad (1)$$

where  $\rho$  is the density,  $\nu$  is the kinematic viscosity and  $\bar{p}$  represents fluid pressure respectively.

As dispersion is known to largely influence by the flow patterns, our aim is to capture the complex dependency between the dispersion coefficient and the reaction parameters in a variety of flow situations such as Poiseuille and Couette flows respectively.

### 2.1 Convection-Diffusion Equation

We have assumed that a Newtonian fluid is flowing through the annular gap of a pipe, also a chemical species is suspended into the solvent which is totally miscible. The species are involved with two different kinds of reactions, viz., kinetic reversible phase exchange and irreversible absorption at inner boundary of annulus. It has been observed that some part of substances stick to the wall of tube while the remaining particles flow along with fluid. Hence to recognize the type of chemical substance, two phases are considered in the modelling of species: mobile phase and immobile phase. Species that flows with fluid is known as mobile phase and that which is fixed at the wall is known as immobile phase. Let the  $\bar{Q}$  is taken as mobile phase concentration and the concentration of the immobile phase be  $\bar{Q}_s$ . If they are in equilibrium state, possess a constant ratio which is termed as partition coefficient, i.e.,

$$\frac{\bar{Q}_s}{\bar{Q}} = \bar{\Omega} \quad (2)$$

where  $\bar{\Omega}$  is known as partition coefficient or a chemical specific constant. If it is impossible to reach the equilibrium state, the following first-order kinetics describes the exchange of the two phases (Ng (2006); Ng and Rudraiah, (2008)):

$$\frac{\partial \bar{Q}_s}{\partial \bar{t}} = K(\bar{\Omega} \bar{Q} - \bar{Q}_s) \quad (3)$$

here  $K$  is rate constant of reversible reaction.

The transport equation that governs the concentration  $\bar{Q}(\bar{r}, \bar{r}, \bar{z})$  is

$$\frac{\partial \bar{Q}}{\partial \bar{t}} + \bar{u}(\bar{r}, \bar{r}) \frac{\partial \bar{Q}}{\partial \bar{z}} = D \frac{\partial^2 \bar{Q}}{\partial \bar{z}^2} + \frac{D}{\bar{r}} \frac{\partial}{\partial \bar{r}} \left( \bar{r} \frac{\partial \bar{Q}}{\partial \bar{r}} \right) \quad (4)$$

where  $D$  considered as constant molecular diffusivity of the solute.

The initial condition is supposed that

$$\bar{Q}(0, \bar{r}, \bar{z}) = G(\bar{r}) \delta(\bar{z}), \quad \bar{b} < \bar{r} < \bar{a} \quad (5)$$

The boundary conditions for the above transport equation is given by (Ng (2006); Ng and Rudraiah, (2008))

$$-D \frac{\partial \bar{Q}}{\partial \bar{r}} - \bar{\Gamma} \bar{Q} = \frac{\partial \bar{Q}_s}{\partial \bar{t}} = K(\bar{\Omega} \bar{Q} - \bar{Q}_s) \text{ at } \bar{r} = \bar{b} \quad (6)$$

$$\frac{\partial \bar{Q}}{\partial \bar{r}} = 0 \text{ at } \bar{r} = \bar{a} \quad (7)$$

where  $G(\bar{r})$  taken as function of  $\bar{r}$ ,  $\delta(\bar{z})$  considered as Dirac delta function. Eq.(6) represents absorbing and reflecting boundary conditions at the inner boundary of the annulus such that both the processes (wall absorption and retention) are not dependent on each other and it is possible to prescribed their rates individually. If we assume the nature of the chemical species is of inert in type w.r.t the wall material ( $\bar{\Gamma} = 0$ ) and there is no storage on the inner wall ( $\bar{Q}_s = 0$ ), the above system reduces to the conventional convection-diffusion equation with simple impermeable boundary conditions, a case extensively studied in the literature (Mazumder and Mondal (2005); Paul and Mazumder (2008)).

The dimensionless quantities proposed for the present problem are listed below.

$$\left. \begin{aligned} Q &= \frac{\bar{Q}}{Q_0}, \quad Q_s = \frac{\bar{Q}_s}{dQ_0}, \quad r = \frac{\bar{r}}{d}, \quad z = \frac{\bar{z}}{d}, \\ t &= \frac{\nu \bar{t}}{d^2}, \quad u = \frac{\bar{u}d}{\nu}, \quad Da = \frac{Kd^2}{D}, \\ \Gamma &= \frac{\bar{\Gamma}d}{D}, \quad \Omega = \frac{\bar{\Omega}}{d}, \quad Sc = \frac{\nu}{D} \end{aligned} \right\} \quad (8)$$

Utilizing Eq. (8), the above system of equations can be rewritten as,

$$\frac{\partial Q}{\partial t} + u(r, t) \frac{\partial Q}{\partial z} = \frac{1}{Sc} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial Q}{\partial r} \right) + \frac{\partial^2 Q}{\partial z^2} \right] \quad (9)$$

with the conditions

$$Q(0, r, z) = G(r) \delta(z), \quad (r_i < r < r_o) \quad (10)$$

$$-\frac{\partial Q}{\partial r} - \Gamma Q = Da(\Omega Q - Q_s) \text{ at } r = r_i \quad (11)$$

$$\frac{\partial Q}{\partial r} = 0 \text{ at } r = r_o \quad (12)$$

Here  $r_o (= 1 / (1 - \eta))$  and  $r_i (= \eta / (1 - \eta))$  are the outer and inner radius of the annular pipe in dimensionless form.  $Sc$  is known as Schmidt number measures the dominance among viscous diffusion and molecular diffusion in mass transfer processes.

The concentration of the immobile phase,  $Q_s$  mentioned in Eq. (11) can be obtained from

$$\frac{\partial}{\partial t} Q_s(z, t) = \frac{Da}{Sc} [\Omega Q(z, r_i, t) - Q_s(z, t)] \quad (13)$$

with  $Q_s(z, 0) = 0$ .

The parameters  $Da$ ,  $\Gamma$  and  $\Omega$  represent the

heterogeneous reactions at the inner boundary of the annular tube. They respectively are the Damköhler number (when  $Da \gg 1$ , it indicates that rate of reaction is higher than rate of diffusion), irreversible absorption parameter (if  $\Gamma \gg 1$ , depletion of huge portion of mass at very short duration) and phase partition ratio or retention parameter (if  $\Omega \ll 1$ , indicates that partition occur more quickly within phases while reverse will be considered for  $\Omega \gg 1$ ).

**2.2 Poiseuille Flow**

Let us consider a pulsatile flow due to the periodic pressure gradient  $\left(-\frac{1}{\rho} \frac{\partial \bar{p}}{\partial z} = P^* \left[1 + \epsilon_p \text{Re}(e^{i\omega_p \bar{t}})\right]\right)$ , and no slip condition holds  $(\bar{u}(\bar{a}, \bar{t}) = \bar{u}(\bar{b}, \bar{t}) = 0)$  at walls of the tube, the velocity  $u(=u_p \text{ (say)})$  in dimensionless form is given by,

$$u_p = u_{ps}(r) + u_{po}(r, t) \tag{14}$$

where

$$u_{ps}(r) = -\frac{P}{4}r^2 + \frac{P}{4}(r_o^2 - r_i^2) \frac{\log r}{\log(r_o / r_i)} + \frac{P}{4 \log(r_o / r_i)} (r_i^2 \log r_o - r_o^2 \log r_i)$$

$$u_{po}(r, t) =$$

$$\text{Re} \left[ i \frac{\epsilon_p P}{\alpha_p^2} \left\{ C_1 J_0(i\sqrt{i}\alpha_p r) + C_2 Y_0(i\sqrt{i}\alpha_p r) - 1 \right\} e^{i\alpha_p^2 t} \right]$$

with

$$C_1 = \frac{Y_0(i\sqrt{i}\alpha_p r_o) - Y_0(i\sqrt{i}\alpha_p r_i)}{J_0(i\sqrt{i}\alpha_p r_i) Y_0(i\sqrt{i}\alpha_p r_o) - J_0(i\sqrt{i}\alpha_p r_o) Y_0(i\sqrt{i}\alpha_p r_i)}$$

$$C_2 = \frac{J_0(i\sqrt{i}\alpha_p r_i) - J_0(i\sqrt{i}\alpha_p r_o)}{J_0(i\sqrt{i}\alpha_p r_i) Y_0(i\sqrt{i}\alpha_p r_o) - J_0(i\sqrt{i}\alpha_p r_o) Y_0(i\sqrt{i}\alpha_p r_i)}$$

$i = \sqrt{-1}$ ;  $\epsilon_p$  is the amplitude and  $\alpha_p = d\sqrt{\frac{\omega_p}{\nu}}$  is the frequency of pressure pulsation.

**2.3 Couette Flow**

Let us consider a pulsatile flow due to the axial movement of outer wall of the annular pipe  $(\bar{u}(\bar{a}, \bar{t}) = U \left[1 + \epsilon_w \text{Re}(e^{i\omega_w \bar{t}})\right], \bar{u}(\bar{b}, \bar{t}) = 0)$  and the pressure gradient is constant  $\left(-\frac{1}{\rho} \frac{\partial \bar{p}}{\partial z} = P^*\right)$ , the flow profile in dimensionless form is given by

$$u_w = u_{ws}(r) + u_{wo}(r, t) \tag{15}$$

where

$$u_{ws}(r) = -\frac{P}{4}r^2 + \frac{P}{4} \frac{(r_o^2 - r_i^2) \log r}{\log(r_o / r_i)} +$$

$$\frac{P}{4} \frac{r_i^2 \log r_o - r_o^2 \log r_i}{\log(r_o / r_i)} + \frac{R_e \log(r / r_i)}{\log(r_o / r_i)} u_{wo}(r, t) = \text{Re} \left[ \left\{ C_1 J_0(i\sqrt{i}\alpha_w r) + C_2 Y_0(i\sqrt{i}\alpha_w r) \right\} e^{i\alpha_w^2 t} \right]$$

with

$$C_1 = \frac{\epsilon_w Y_0(i\sqrt{i}\alpha_w r_i)}{J_0(i\sqrt{i}\alpha_w r_i) Y_0(i\sqrt{i}\alpha_w r_o) - J_0(i\sqrt{i}\alpha_w r_o) Y_0(i\sqrt{i}\alpha_w r_i)}$$

$$C_2 = \frac{-\epsilon_w J_0(i\sqrt{i}\alpha_w r_i)}{J_0(i\sqrt{i}\alpha_w r_i) Y_0(i\sqrt{i}\alpha_w r_o) - J_0(i\sqrt{i}\alpha_w r_o) Y_0(i\sqrt{i}\alpha_w r_i)}$$

$U$ , represents the steady component of velocity due to the movement of the outer wall,  $\epsilon_w$  is the amplitude and  $\alpha_w = d\sqrt{\frac{\omega_w}{\nu}}$  is the frequency of the wall oscillation.  $P = \frac{d^3 P^*}{\nu^2}$  is the Poiseuille number and  $R_e = \frac{ud}{\nu}$  is the Reynolds number. ‘Re (.)’ indicates the real part of a complex number.

**3. MOMENT EQUATIONS**

Following Aris (1956), the  $q^{\text{th}}$  moment of solute distribution (within a mobile phase) in the longitudinal direction as

$$Q^{(q)}(t, r) = \int_{-\infty}^{+\infty} z^q Q(t, r, z) dz \tag{16}$$

Also the  $q^{\text{th}}$  moment for solute distribution (within an immobile phase) can be defined as

$$Q_s^{(q)}(t) = \int_{-\infty}^{+\infty} z^q Q_s(z, t) dz \tag{17}$$

Using Eqs. (16) and (17), in Eqs. (9)- (13) become

$$\frac{\partial Q^{(q)}}{\partial t} - \frac{1}{Sc} \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial Q^{(q)}}{\partial r} \right) = q u(r, t) Q^{(q-1)} + \frac{1}{Sc} q(q-1) Q^{(q-2)} \tag{18}$$

With

$$\left. \begin{aligned} Q^{(q)}(0, r) &= \begin{cases} G(r) & \text{for } q = 0 \\ 0 & \text{for } q > 0 \end{cases} \\ -\frac{\partial Q^{(q)}}{\partial r} - \Gamma Q^{(q)} &= Da[\Omega Q^{(q)} - Q_s^{(q)}] \quad \text{at } r = r_i \\ \frac{\partial Q^{(q)}}{\partial r} &= 0 \quad \text{at } r = r_o, \end{aligned} \right\} \tag{19}$$

It will be apparent that  $G(r) = 1$  for  $r_i < r < r_o$ .

In the immobile phase the equation for the moments of the mass distribution is

$$\frac{d}{dt} Q_s^{(q)} = \frac{Da}{Sc} \left[ \Omega Q^{(q)}(t, r_i) - Q_s^{(q)} \right] \quad (20)$$

with  $Q_s^{(q)}(0) = 0$ .

An angle bracket is employed to symbolize the averaging of the cross-sectional area of annulus, as

$$\langle Q^{(q)}(t) \rangle = \frac{2}{r_o^2 - r_i^2} \int_{r_i}^{r_o} r Q^{(q)}(t, r) dr \quad (21)$$

Now with the help of Eq. (21), the integral moment Eqs. (18) and (19) can take the form as

$$\begin{aligned} \frac{d}{dt} \langle Q^{(q)} \rangle &= \frac{1}{Sc} \frac{2 r_i}{r_o^2 - r_i^2} \left[ \Gamma Q^{(q)}(t, r_i) \right. \\ &\quad \left. + Da \left( \Omega Q^{(q)}(t, r_i) - Q_s^{(q)}(t) \right) \right] + \\ &\quad q \langle u(r, t) Q^{(q-1)} \rangle + \frac{1}{Sc} q(q-1) \langle Q^{(q-2)} \rangle \end{aligned} \quad (22)$$

with,

$$\begin{aligned} \langle Q^{(q)}(0) \rangle &= 1 \quad \text{for } q = 0 \\ &= 0 \quad \text{for } q > 0 \end{aligned} \quad (23)$$

The distribution of solute concentration can be describe with respect to the central moments as follows

$$\mu_q(t) = \frac{\int_{r_i}^{r_o} \int_0^{2\pi} \int_{-\infty}^{+\infty} r(z - z_g)^q Q dr d\theta dz}{\int_{r_i}^{r_o} \int_0^{2\pi} \int_{-\infty}^{+\infty} r Q dr d\theta dz} \quad (24)$$

Where

$$z_g = \frac{\iiint z Q dv}{\iiint Q dv} = \frac{\langle Q^{(1)} \rangle}{\langle Q^{(0)} \rangle}$$

is the first moment or centroid of the solute distribution.  $\langle Q^{(0)} \rangle$  represents the actual amount of solute in the bulk flow.

For values  $q = 2, 3$  and  $4$  in Eq. (24), the second, third and fourth order central moments are:

$$\left. \begin{aligned} \mu_2(t) &= \frac{\langle Q^{(2)} \rangle}{\langle Q^{(0)} \rangle} - z_g^2, \\ \mu_3(t) &= \frac{\langle Q^{(3)} \rangle}{\langle Q^{(0)} \rangle} - 3z_g \mu_2 - z_g^3, \\ \mu_4(t) &= \frac{\langle Q^{(4)} \rangle}{\langle Q^{(0)} \rangle} - 4z_g \mu_3 - 6z_g^2 \mu_2 - z_g^4, \end{aligned} \right\} \quad (25)$$

When analyzing the phenomena of dispersion, [Aris \(1956\)](#) revealed the physical significance of an integral moments having concentration mentioned in Eq.(25). The integral moment Eq.(18), represents sequence of inhomogeneous equations

for  $q = 0, 1, 2, 3, \dots$ ; and can be solved for sufficiently excessive values of  $q$  for the distribution to be developed at any degree of accuracy. As finally distribution leads to normality so the first two moments are eventually enough for the description of distribution where the third and fourth moments should be zero. First three and four moments provide very significant information about the progress of dispersion. The complete nature of the slug can be efficiently described by those integral moments:

The zeroth order moment provides the whole area under the distribution curve, which in other way relating to the overall mass of the mobile phase. Observing at the initially located source, first order moment is useful to find the position of the center of mass distribution. Among them the variance or second order central moment ( $\mu_2$ ) about mean is the most important since the rate of change of  $\mu_2$  with respect to time is same as dispersion coefficient. According to [Aris \(1956\)](#), the form of the apparent dispersion coefficient  $D_c$  proposed as

$$D_c = \frac{d\mu_2}{dt} \quad (26)$$

The coefficient of skewness  $\nu_2 (= \mu_3 / \mu_2^{3/2})$  and kurtosis  $\nu_3 (= \mu_4 / \mu_2^2 - 3)$  are also essential for finding the solution of mean concentration distribution in the axial direction.

#### 4. NUMERICAL SOLUTION

A standard finite difference method (FDM) constructed on Crank-Nicolson implicit scheme has been implemented for the solution of differential Eqs. (18) and (20) with initial and boundary conditions in Eq. (19) as of difficulties in moment equation for  $q > 1$ . The entire width of the annulus is divided into  $(M - 1)$  equal slice of mesh size  $\Delta r$ , denoted by grid point  $j$ . Thus the inner and outer walls of the annulus are addressed by  $j = 1$  and  $j = M$  individually, i.e.,  $r_j = r_i + (j - 1) \times \Delta r$ . The time is indexed by the grid point  $i$  where each of the step size is assumed to be  $\Delta t$ . The general form of time discretization is  $t_i = \Delta t \times (i - 1)$ , hence the initial time  $t = 0$  is found for fixed  $i = 1$ .  $Q^{(q)}(i, j)$  represent the particular values of  $Q^{(q)}$  at the grid points  $i$  and  $j$  respectively. The proposed FDM scheme reduce the differential equations into a tri-diagonal coefficient matrices as:

$$\begin{aligned} P_j Q^{(q)}(i+1, j+1) + Q_j Q^{(q)}(i+1, j) + \\ R_j Q^{(q)}(i+1, j-1) = S_j, \end{aligned} \quad (27)$$

where  $P_j$ ,  $Q_j$ ,  $R_j$  and  $S_j$  are termed as element of matrix.

The finite difference form of the initial condition is,

$$\begin{aligned} Q^{(q)}(1, j) &= 1 \quad \text{for } q = 0 \\ &= 0 \quad \text{for } q > 0 \end{aligned} \quad (28)$$

and that of boundary conditions are

$$\begin{aligned} Q^{(q)}(i+1, 0) &= Q^{(q)}(i+1, 2) + 2\Delta r(\Gamma + Da\Omega) \\ &\quad Q^{(q)}(i+1, 1) - 2\Delta r Da Q_s^{(q)}(i+1), \end{aligned} \quad (29)$$

(at the surface of the inner cylinder)

$$Q^{(q)}(i+1, M+1) = Q^{(q)}(i+1, M-1),$$

(at the surface of the outer cylinder)

where  $Q_s^{(q)}(i)$  can be computed from the relation

$$Q_s^{(q)}(i+1) = \frac{\left[ Q_s^{(q)}(i) + \frac{Da}{Sc} \Delta t \Omega Q^{(q)}(i+1, 1) \right]}{\left[ 1 + \frac{Da}{Sc} \Delta t \right]} \quad (30)$$

with the initial condition  $Q_s^{(q)}(0) = 0$ .

Utilizing the Thomas algorithm (Anderson, Tannehill and Pletcher (1984)), the solution of Eqs. (27) - (30) has been done by means of a MATLAB code. The computation steps are as: (i) From Eqs. (14) and (15), the velocity distributions  $u(r, t)$  of Poiseuille and Couette flows are estimated first. (ii) utilizing the results of  $u(r, t)$  obtained from the previous step at every grids, the solution of the concentration  $Q^{(q)}$  is computed from the moment Eq. (18). (iii) this step will find the solutions of  $Q_s^{(q)}$  from Eq. (20) as we already know the values of  $Q^{(q)}$ . and (iv) lastly, using Simpson's one-third rule, cross sectional average  $\langle Q^{(q)} \rangle$  is calculated from Eq. (21) as the solutions of  $u(r, t)$ ,  $Q^{(q)}$  and  $Q_s^{(q)}$  are all known at the matching grid positions.

Numerical computations have been executed for steady, oscillatory and combined flow situations by their individual effect on dispersion process under the variation of different parameters and velocity distributions. We know the Crank-Nicolson implicit scheme is unconditionally stable for arbitrarily any fixed values of  $\Delta t / (\Delta r)^2$ , also suitably small mesh size ( $\Delta r = (r_o - r_i) / (M - 1)$ ) of spatial and temporal ( $\Delta t = 0.00001$ ) discretization have been confirmed an accuracy of  $10^{-5}$  in the results.

In all the cases we have taken  $\alpha_p = \alpha_w = 5$ ,  $\epsilon_p = \epsilon_w = 1$ ,  $Re = P = 1$ ,  $\Omega = 0.5$ ,  $Sc = 10^3$ . Both the time and space intervals are needed to be small to observe the pulsatile behavior in dispersion and to maintain the accuracy of the outcomes.

## 5. DISTRIBUTIONS OF MEAN CONCENTRATION

According to very popular works of Taylor (1953), for a shear-dependent flow, the distribution of solute concentration is centered on a point which travels with the mean speed of the flow. Taylor dispersion process describes an asymptotic stage for transport of solute across transversely restricted flow region. The mean concentration distribution in the longitudinal direction forms a Gaussian like distribution during the transport process. When the major effect is convection in comparison to dispersion, it is estimated that resulting curve will considered nearly Gaussian (Levenspiel and Smith (1957)) then the concentration might be characterized by way of series in Hermite polynomials. The Aris's method of moment is useful for finding the central moments, again using higher order central moments it is likely to approximate the average axial concentration distribution  $Q_m(z, t)$  of tracer across the flow region via help of Hermite polynomial representation of non-Gaussian curves (Mehta, Merson and McCoy (1974)). The cross-sectional mean concentration  $Q_m(z, t)$  is defined as

$$Q_m(z, t) = \langle Q^{(0)}(t) \rangle e^{-\lambda^2} \sum_{n=0}^{\infty} a_n(t) H_n(\lambda) \quad (31)$$

where  $\lambda = (z - z_g) / \sqrt{2\mu_2}$ ,  $z_g = \frac{\langle Q^{(1)} \rangle}{\langle Q^{(0)} \rangle}$  and  $H_i$

represents the Hermite polynomial and is satisfying the recurrence relation as

$$H_{i+1}(\lambda) = 2\lambda H_i(\lambda) - 2i H_{i-1}(\lambda), \quad i = 0, 1, 2, \dots$$

and  $H_0(\lambda) = 1.0$

The coefficients  $a_i$ 's are

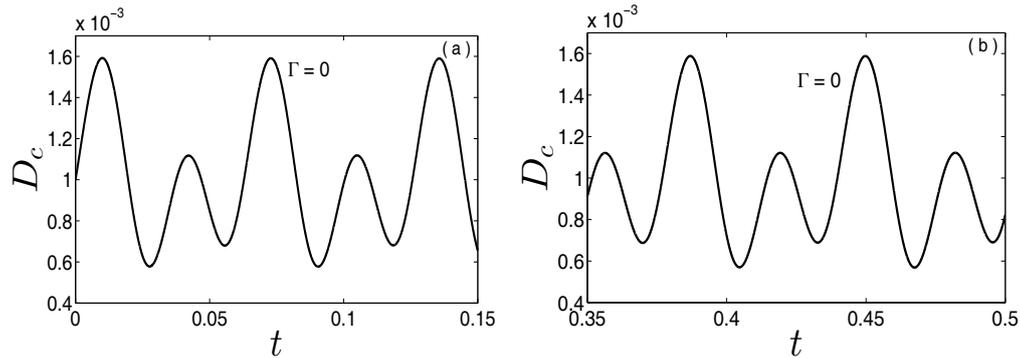
$$\begin{aligned} a_0 &= 1 / (2\pi\mu_2)^{1/2}, \quad a_1 = a_2 = 0, \\ a_3 &= 2^{1/2} a_0 v_2 / 24, \quad a_4 = a_0 v_3 / 96 \end{aligned} \quad (32)$$

Thus, utilizing the values of various central moments obtained from Eq. (25), the mean concentration distribution of chemical species in the axial direction can be estimated from Eq. (31) at any fixed time.

## 6. RESULTS AND DISCUSSION

To study the longitudinal dispersion of reactive material flowing through an annular pipe, a pulsatile nature of Poiseuille and Couette flows are considered due to its versatile applications. In this article, a dispersion study is carried out using the Aris-Barton's methodology and the following cases were examined to verify the accuracy of the numerical scheme:

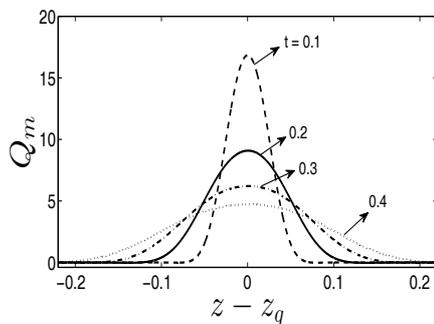
Case-I: If  $Da = 0$ , the present problem can be reduced to the study of S. Paul (2011) when the flow unsteadiness is due to the upper wall oscillation. To this end, the model responses outlaid in Fig. 2 displays complete agreement with those obtained in the study of solute dispersion of S. Paul



**Fig. 2.** Variation of the dispersion coefficient  $D_c$  with time when  $Da = 0$ ,  $\eta = 0.1$ ,  $\alpha_w = 10$ , (a) for small times; (b) for large times.

(2011) without reversible reaction. (see Figs. 2(a, b) totally coincide with Figs. 7(a, b) in (S. Paul (2011) when irreversible reaction parameter value is 0).

Case-II: If the inner boundary of annular pipe is inert, the present model becomes a circular pipe model when  $\eta \rightarrow 0$ , a case studied by Mazumder and Das (1992) under time dependent poiseuille flow. Figure 3 shows the axial distribution of mean concentration due to combined flow when  $\Gamma = 0$ ,  $Da = 0$  and  $\eta \rightarrow 0$ , etc., qualitatively agrees the result of Mazumder and Das (1992) for pipe flow, such that, the increase of dispersion times lead to decrease the peak of the distribution. However, the quantitative differences realized in Fig. 3 is attributed to differing normalization scales adopted in the present study.



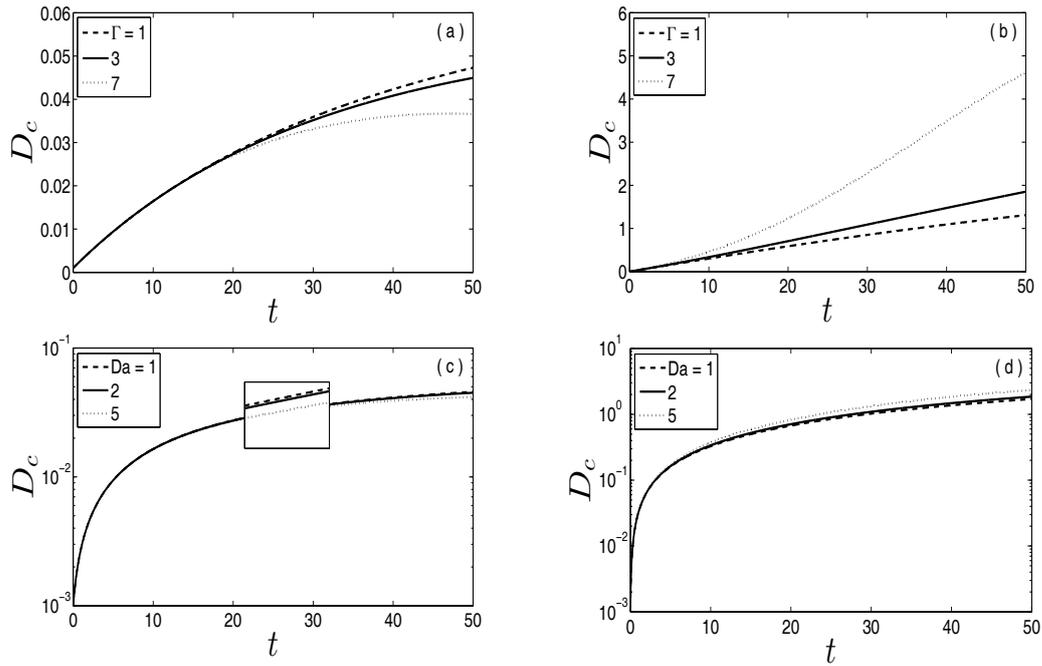
**Fig. 3.** Axial distribution of mean concentration with time for a combined flows under periodic pressure gradient when  $Da = 0$ ,  $\Gamma = 0$ ,  $\alpha_p = 1$ ,  $\epsilon_p = 1.5$ , and  $\eta = 0$ .

Variation of dispersion coefficient with respect to time is shown in Fig. 4 for a variety of steady flows with different values of the reaction parameters. A wide range of time is considered to track the asymptotic approachment of the dispersion coefficient. As already mentioned earlier two types of flow patterns (i) flow due to pressure gradient, (ii) flow due to the axial movement of the outer cylinder and two types of reaction parameters (i) Damköhler number  $Da$ , and (ii) irreversible absorption parameter  $\Gamma$  have been considered for

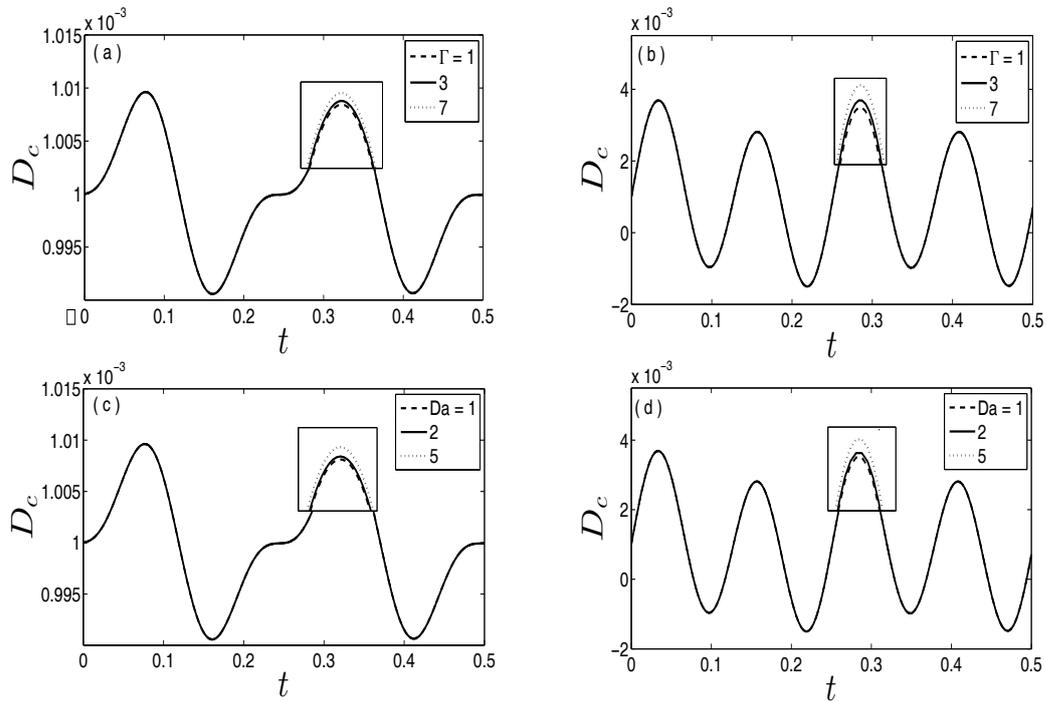
the present study giving rise to an array of figures with two rows and two columns. Profiles in the first column of Fig. 4 are for flow because of pressure gradient while next column describes nature of dispersion coefficient when the flow is due to movement of the upper wall of the annulus respectively. The two successive rows explain respectively the effects of  $\Gamma$  and  $Da$  on the dispersion coefficient in various flow circumstances as mentioned above.

From Fig. 4, initially, dispersion coefficient is found to increase with time in a significant manner though as time goes the increments get slower in any flow situation. Flow due to the steady component of wall oscillation, Figs. 4(b, d) show that dispersion coefficient increases with respect to both reversible and irreversible reaction parameters. It is remarkable to note that for flow driven by pressure gradient,  $D_c$  is increasing with  $\Gamma$  and  $Da$  for times  $t < 12$  and  $t < 10$  respectively. Again, after that critical times, for both reversible and irreversible boundary reactions, the increase of reaction parameters may lead to reduce the value of the dispersion coefficient. [This fact can be realized further from Fig. 10]

For the case of purely oscillatory flow, time assessment of dispersion coefficient is shown in Figs. 5, and 6 for small and large time respectively. During the initial time, dispersion coefficient with the variation of reaction parameters is found to be irrespective of the flow situations (Fig. 5). It has shown in Fig. 5, in any flow situation the increase of reaction parameters that are associated with the heterogeneous irreversible and reversible reactions (i.e.,  $\Gamma$  and  $Da$ ) on the inner tube wall may lead to increase the dispersion coefficient. It is worthy to note that the response of dispersion coefficient with reaction parameter should not be considered as final, situation may be different depending on other factor such as duration of time, reaction strength, radius ratio etc. This fact can be partially realized later from Fig. 9. The gradual development of a second peak in the dispersion curve is noticeable from any of the Fig. 5. For pressure driven flow the peak is almost suppressed; whereas it is partially expressed in outer wall driven flow. When the time is large,



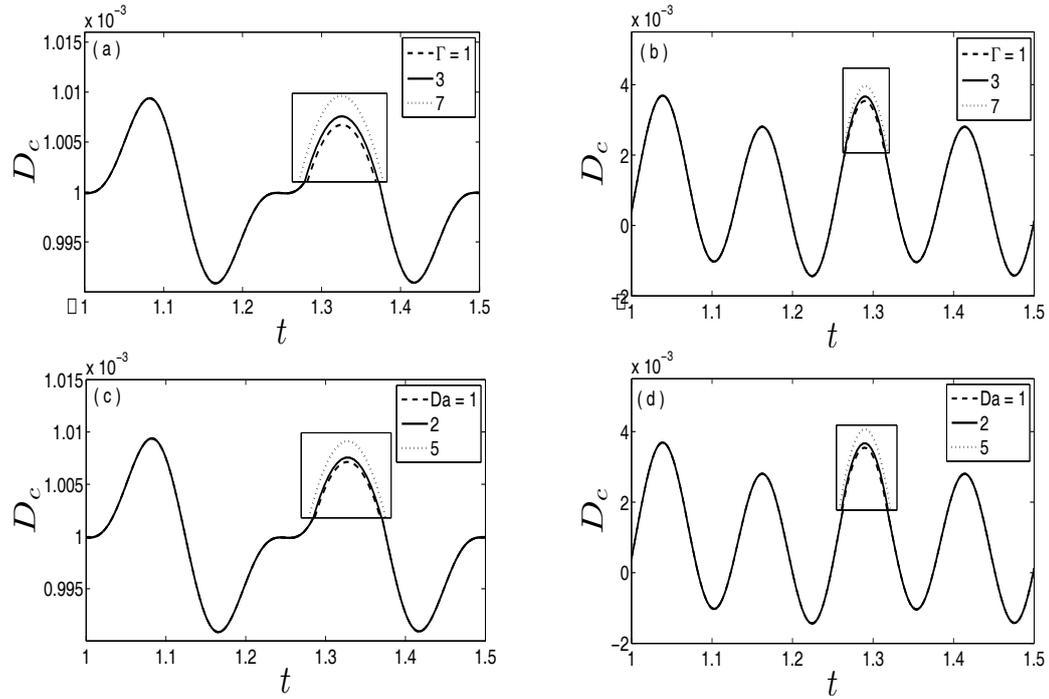
**Fig. 4.** For steady flow, variation of the dispersion coefficient with time for two different kinds of reaction parameters and also for two different kinds of flow. (a, b) Effect of heterogeneous irreversible reaction ( $\Gamma$ ) when  $Da = 2$ , (c, d) effect of heterogeneous reversible reaction ( $Da$ ) when  $\Gamma = 3$ . (a, c) For flow driven by pressure gradient, (b, d) for flow driven by axial motion of the outer wall of the annulus.



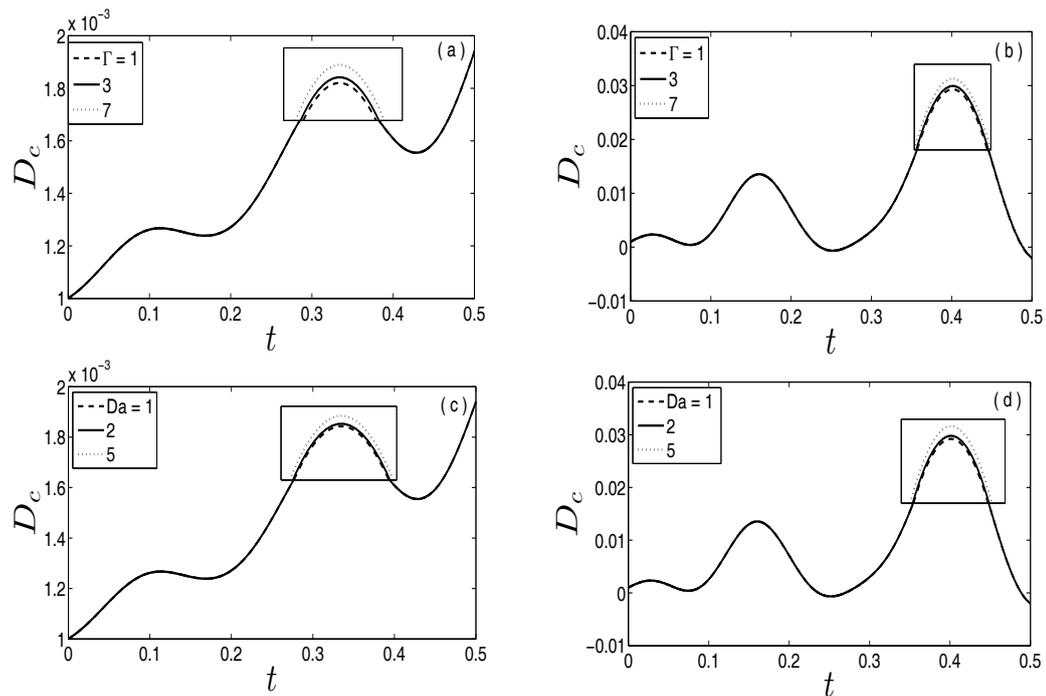
**Fig. 5.** At small times, variation of the dispersion coefficient against time for purely oscillatory flow for different reaction parameters and velocity profiles. Other descriptions are as in Fig. 4.

somewhat similar qualitative effects of different reaction parameters on the dispersion coefficient can be seen from Fig. 6.

For combined flow, the response of dispersion coefficient with time (small and large) are displayed in Figs.7 and 8 separately. The arrangement of the



**Fig. 6.** Same as Fig. 5, but at large times.



**Fig. 7.** For combined flow, variation of the dispersion coefficient against time at small times for different reaction parameters and velocity profiles. Other descriptions are as in Fig. 4.

figures is same as the previous figures. It can be seen from Fig. 7 that, similar to the case of purely oscillatory flow, in this case also dispersion coefficient indicates an increasing trend with the growth of reaction parameters relating to boundary reactions. More vivid effects of the reaction parameters can be noted in Fig. 8, though the qualitative nature of the dispersion coefficient remains the same as in initial time (Fig. 7) under the

variation of the reaction parameters. Also, responses of the dispersion coefficient seem to be more sensitive at large time, i.e., at large time effects are more pronounced.

The effect of radius ratio  $\eta$  on solute dispersion has been demonstrated in Fig. 9 when the combined effect of both steady and oscillatory velocity components are assumed. Fig. 9(a) is due to

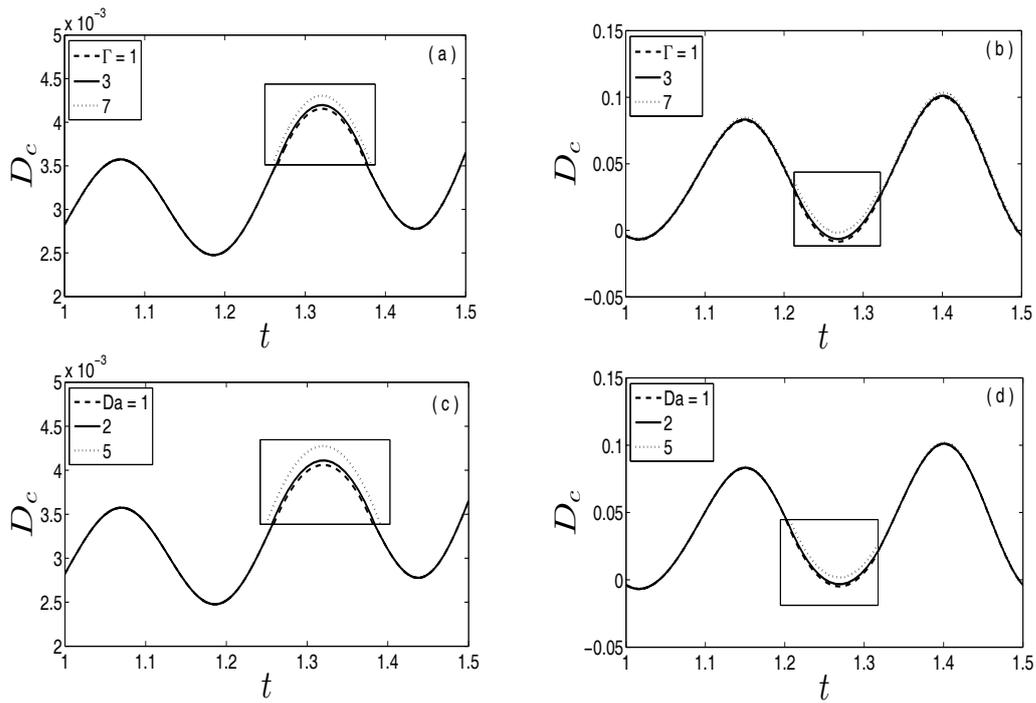


Fig. 8. Same as Fig. 7 but at large times.

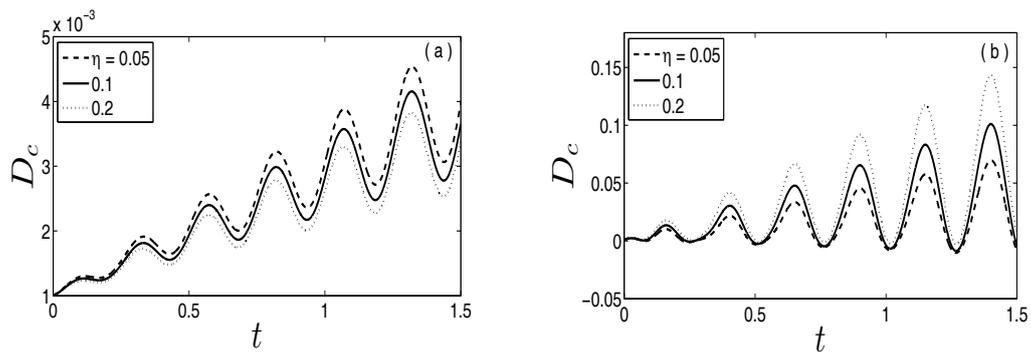


Fig. 9. Temporal variation of dispersion coefficient  $D_c$  for various values of radius ratio  $\eta$  under different types of unsteady flow situations where unsteadiness is caused by the (a) sole oscillation of the pressure gradient and (b) sole oscillation of the outer wall of annular tube, when  $\Gamma = 3$  and  $Da = 2$ .

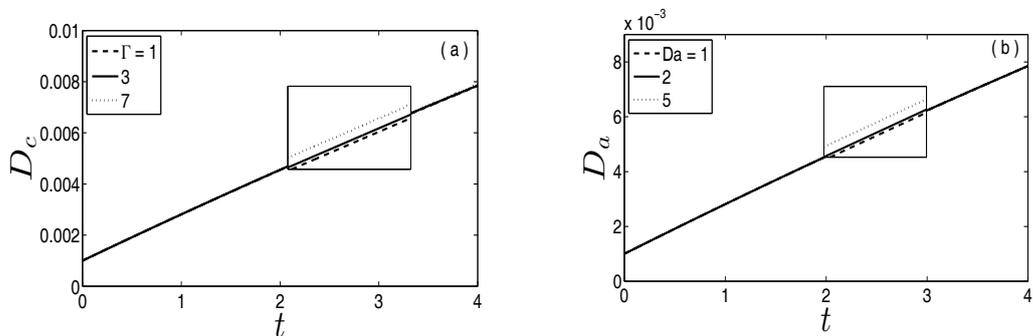
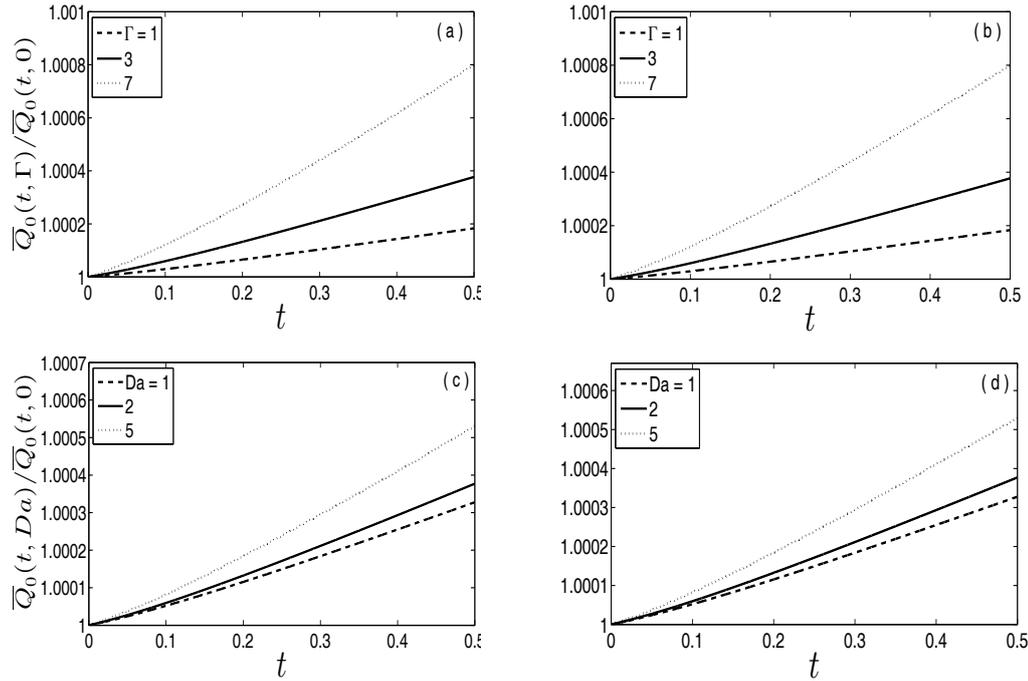


Fig. 10. Flow driven by steady pressure gradient, variation of the dispersion coefficient with time for two different kinds of reaction parameters, (a): effect of heterogeneous irreversible reaction ( $\Gamma$ ) when  $Da = 2$ , (b): effect of heterogeneous reversible reaction ( $Da$ ) when  $\Gamma = 3$ .



**Fig. 11. (a, b) Dimensionless mass as a function of heterogeneous irreversible reaction parameter  $\Gamma$  against time, (c, d) dimensionless mass for the reversible reaction parameter  $Da$  against time. Other descriptions are as in Fig. 4.**

periodic pressure gradient such that larger values of  $\eta$  makes a significant decrements on  $D_c$ . Also large values of  $\eta$  leads to increase the value of dispersion coefficient when the outer wall movement of an annular pipe is the reason of flow pulsation (Fig. 9(b)). Hence from the present model, the relation among  $D_c$  and  $\eta$  are completely depending on the flow geometry.

When  $q = 0$ , Eq. (22) becomes,

$$\begin{aligned} \langle Q^{(0)}(t, \Gamma, \Omega, Da, \dots) \rangle &= \frac{1}{Sc} \frac{2r_i}{r_o^2 - r_i^2} \Gamma \int Q^{(0)}(t, r_i) dt \\ &+ \frac{1}{Sc} \frac{2r_i}{r_o^2 - r_i^2} Da \left[ \Omega \int Q^{(0)}(t, r_i) dt - \int Q_s^{(0)}(t) dt \right] \end{aligned} \quad (33)$$

Here  $Q^{(0)}(t, r_i)$  and  $Q_s^{(0)}(t)$  can be found from the solution of Eqs.(18) and (20) respectively. Eq. (33) signifies the actual mass of the reactive species where the 1<sup>st</sup> and 2<sup>nd</sup> term of the right side of Eq.(33) represent the effects of irreversible boundary absorption and phase exchange respectively. When  $\Gamma = Da = 0$ ,  $\langle Q^{(0)} \rangle = 1$ , representing total mass in the annular gap is constant with time. It can be seen from Fig.11 that

dimensionless mass  $\frac{\langle Q^{(0)}(t, \Gamma, \dots) \rangle}{\langle Q^{(0)}(t, 0, \dots) \rangle}$  and  $\frac{\langle Q^{(0)}(t, Da, \dots) \rangle}{\langle Q^{(0)}(t, 0, \dots) \rangle}$  are increasing functions of the

corresponding parameter and time  $t$ .

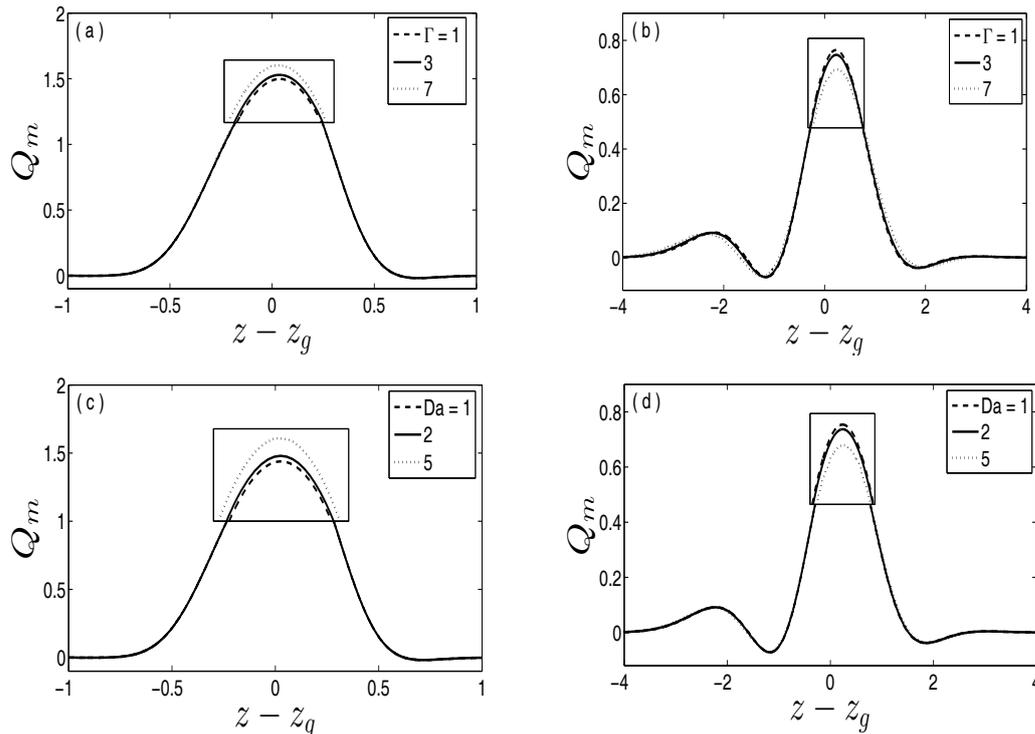
For steady flow, the mean of the concentration distribution in the axial direction has been shown in Fig. 12. Flow driven by pressure gradient, the concentration curves head may rise with the augmentation of the both  $\Gamma$  and  $Da$ , the respective irreversible and reversible parameters for heterogeneous reactions at the inner boundary. An opposite scenario has been observed from the flow driven by the axial motion of the outer cylinder, such as, stronger  $\Gamma$  or  $Da$  both lead to a fall of the peak of the concentration profile.

## 7. CONCLUSIONS

The paper aims to investigate the effect of heterogeneous reaction on the dispersion coefficient through an annulus. As we know the flow conditions may significantly control the dispersion process, both Poiseuille and Couette flow are taken into consideration for analysis. The coupled effects of the reaction parameters on the dispersion coefficient are examined in two different flow conditions.

The study disclose the following attributes of transport of species:

- i. For all times,  $D_c$ , on account of steady part of outer wall oscillation is an increasing function of both  $\Gamma$  and  $Da$  respectively.
- ii. At small time,  $D_c$ , owing to steady part of periodic pressure gradient is an increasing function of both  $\Gamma$  and  $Da$  respectively.



**Fig. 12.** Axial distribution of mean concentration for two different kinds of steady flows with different values of the reaction parameters at a fixed time,  $t = 5$ . Other descriptions are as in Fig. 4.

However, after that critical time  $D_c$  is decreased by the reaction parameters.

- iii. In any flow situation dispersion coefficient due to purely oscillatory as well as combined flows are increased by heterogeneous irreversible and reversible reactions at the inner tube wall.
- iv. In a Poiseuille flow,  $D_c$  is decreased by increasing radius ratio of the annular tube which in contrast of the results obtained from Couette flow.
- v. In a Couette flow, both  $\Gamma$  or  $Da$  lead to a fall of the head of the concentration profile. However, a reverse effect has been captured for Poiseuille flow.

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