Influence of nonlinear chemical reactions on the transport coefficients in oscillatory Couette flow

Swarup Barik and D. C. Dalal
Department of Mathematics, IIT Guwahati, Guwahati, India
E-mail: s.barik@iitg.ernet.in, durga@iitg.ernet.in

Abstract. A multiple-scale method of averaging is applied to the study of transport of a chemical species in oscillatory Couette flow where the species may undergoes a reversible phase exchange with the boundary wall and nonlinear chemical reactions both within the fluid and at the boundary wall. Analytical expressions are obtained for transport coefficients. The results shows how the transport coefficients are influenced by the reversible phase exchange reaction kinetics and the rate and degree of the nonlinear decay chemical reaction.

1. Introduction
Transport of a solute in a fluid flow has several important applications in diverse fields such as biology, chemistry, chromatography and environmental fluid mechanics. Taylor [9] first studied theoretically as well as experimentally the transport of a solute dissolved in a fluid flowing through a circular pipe of constricted diameter. Since then, this mechanism has been termed as “Taylor dispersion”. In the system, reaction may take place in the bulk flow (mobile phase) and at the sorbet boundaries (immobile phases). It may be reversible or irreversible in nature and it may also be classified as linear or nonlinear.

Dispersion in oscillatory Couette flow without reaction has been studied by Mazumder and co-workers [1, 5] using a modified moments method. Solute transport in oscillatory Couette flow with linear phase exchange reaction has been analysed by Ng and Bai [4]. Revelli and Ridolfi [7, 8], Paul and Mazumder [6] have shown the effects of nonlinear chemical reactions on solute transport. In spite of its environmental and industrial applications, less attention has been paid to the study of nonlinear reactions on solute transport.

The main purpose of this study is to explore the effects of nonlinear chemical decay phenomena on transport coefficients in an oscillatory Couette flow. A 2-D mathematical model is formulated by considering the effects of diffusion, advection, decay and a phase exchange kinetics between mobile and immobile phases. In the present work, nonlinear decay reaction terms are included in both in mobile and immobile phases and this is a generalization of the work of Ng and Bai [4]. This study may help to model shear-driven flows encountered in micro motors, micro channels and other micro fluidic systems.

2. Problem under consideration
A laminar, one-dimensional plane Couette flow between two infinite parallel flat walls with a separation width $h$ is considered. The lower boundary at $y = 0$ is assumed to be stationary
whereas the upper boundary at $y = h$ oscillates in its own plane with a prescribed velocity

$$u(h, t) = U[1 + \phi Re(e^{-i\omega t})],$$

where $U$ is the steady component of the velocity of the upper boundary, $\phi$ is a factor such that $\phi U$ is the amplitude of the oscillatory velocity component, $\omega$ is the angular frequency of the plate oscillation, $t$ is time and $Re$ stands for real part. The velocity profile of the flow can be taken as (Ng and Bai [4])

$$u(y, t) = u_s + Re(u_w e^{-i\omega t}),$$

where $u_s(y) = U y / h$ and $u_w(y) = U \phi \sin \frac{\pi y}{h}$ are the steady and oscillatory components of the velocity field respectively. Here $\sigma^2 = i \omega / \nu$ or $\sigma = (1 + i) / \delta$ and $\delta = \sqrt{2 \nu / \omega}$, where $\nu$ is the kinematic viscosity of the fluid.

The chemical considered in this study is assumed to be completely miscible in the fluid and would undergo a reversible sorptive phase exchange across the fluid-lining interface. It is possible that in the lining the chemical exists in a form different from that in the flowing fluid. To distinguish between the forms of the chemical that exist in the fluid and in the lining, we referred to them as the mobile and the immobile phases, respectively. Because of reversible phase exchange reaction, the chemical sticks into immobile phase from mobile phase and reversely release into mobile phase from immobile phase. It is also assumed that the chemical undergoes nonlinear decay reaction both in mobile and the immobile phases and at equilibrium stage, these two phases will have their concentrations in a fixed ratio

$$C_s / C = \alpha,$$

where $C$ is the concentration (mass of chemical per bulk volume of fluid) of the mobile phase, $C_s$ is the concentration (mass of chemical per surface area of wall) of the immobile phase and $\alpha$ the partition coefficient having the dimension of length.

If the equilibrium is not attained, the phase exchange kinetics along with nonlinear decay chemical reaction (defined by $\Delta_s$) generally takes place either in forward or in backward direction (Paul and Mazunder [6]) according to

$$\frac{\partial C_s}{\partial t} = k(\alpha C - C_s) + \Delta_s,$$

where $k$ is the reversible reaction rate constant.

The problem for the transport of the chemical can be formulated as follows:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2} + D \frac{\partial^2 C}{\partial y^2} + \Delta, \quad 0 < y < h,$$

(1)

where $D$ is the molecular diffusivity of the chemical in the fluid assumed to be constant and $\Delta$ represents the effect of nonlinear chemical reaction occurring in the bulk flow.

The corresponding reaction rates, $\Delta$ and $\Delta_s$ are prescribed according to the power laws,

$$\Delta = -\lambda C^n, \quad \Delta_s = -\lambda_s C_s^n, \quad (i = 1, 2),$$

where $\lambda$ and $\lambda_s$ are the reaction rate constants for the mobile and immobile phases respectively and $n$ and $m$ are the corresponding degrees of nonlinearity.

The boundary conditions for (1) are taken as

$$D \frac{\partial C}{\partial y} = \frac{\partial C_s}{\partial t} = k_1(\alpha_1 C - C_s) - \lambda_{s1} C_{s1}^n, \quad y = 0,$$

$$-D \frac{\partial C}{\partial y} = \frac{\partial C_{s2}}{\partial t} = k_2(\alpha_2 C - C_{s2}) - \lambda_{s2} C_{s2}^m, \quad y = h.$$

(2) (3)

The subscripts 1 and 2 are used to denote quantities associated with the lower and upper boundaries.
3. Assumptions for asymptotic analysis

Homogenization technique proposed by Mei et al. [2] has been applied in this study. It is assumed that a sufficiently long time has passed since the discharge of the chemical into the flow so that the length scale for the axial spreading of the chemical cloud is much greater than the channel depth, and $\epsilon = h/L(\ll 1)$ used as the perturbation parameter. Along with two different length scales $h$ and $L$, three distinct time scales have also been considered for lateral diffusion, advection/reaction and axial diffusion (Ng [3]). Their ratios are

$$T_0:T_1:T_2 = 1:\frac{1}{\epsilon}:\frac{1}{\epsilon^2}.$$ 

Based on these time scales, fast, medium and slow time variables have been introduced accordingly as follows

$$t_0 = t, \quad t_1 = \epsilon t, \quad t_2 = \epsilon^2 t.$$ 

The original time derivative becomes, according to the chain rule:

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2}.$$ 

Dependent variables are expanded in power series to carry on perturbation analysis:

$$C = C^{(0)} + \epsilon C^{(1)} + \epsilon^2 C^{(2)} + O(\epsilon^3),$$

$$C_{si} = C_{si}^{(0)} + \epsilon C_{si}^{(1)} + \epsilon^2 C_{si}^{(2)} + O(\epsilon^3), \quad (i = 1, 2).$$

By perturbation analysis, 1-D transport equation has been obtained that describes the averaged behavior of the 2-D phenomenon.

4. Transport coefficients

Let us introduce the following normalised variables

$$\hat{C}^{(0)} = \frac{C^{(0)}}{C_0}, \quad \hat{\alpha}_1 = \frac{\alpha_1}{h}, \quad \hat{\alpha}_2 = \frac{\alpha_2}{h}, \quad \hat{\beta}_1 = \frac{\beta_1}{D}, \quad \hat{\beta}_2 = \frac{\beta_2}{D}, \quad Da_1 = \frac{k_1 h^2}{D}, \quad Da_2 = \frac{k_2 h^2}{D}, \quad \hat{\lambda} = \frac{\lambda}{k_s C_0^{n-1}},$$

$$\hat{\lambda}_{s1} = \frac{\lambda_{s1}}{k_1 h^{m-1} C_0^{m-1}}, \quad \hat{\lambda}_{s2} = \frac{\lambda_{s2}}{k_2 h^{m-1} C_0^{m-1}}, \quad \hat{\sigma} = \sigma h, \quad \hat{\eta} = \eta h, \quad \hat{\delta} = \frac{\delta}{h},$$

where $\beta_j = -\frac{\omega k_j \eta_j}{D}$, $(j = 1, 2$ and $i = \sqrt{-1})$. The Damkohler number $Da$ is the ratio of phase exchange rate to the diffusion rate. Here in the expression of $\hat{\lambda}$, it is considered that $k_s = k_1$ only when the lower boundary is sorbing (Case 1), $k_s = k_2$ only when the upper boundary is sorbing (Case 2) and without loss of generality $k_s = k_1 = k_2$ when both boundaries are sorbing (Case 3). Using this normalised variables, the effective transport equation can be obtained by perturbation analysis of (1) - (3) as

$$\frac{\partial \hat{C}^{(0)}}{\partial t} = \left[ \frac{D}{R} + \hat{D}_{T_s} \frac{U^2 h^2}{D} + \hat{D}_{T_w} \frac{U^2 h^2}{D} \right] \frac{\partial^2 \hat{C}^{(0)}}{\partial x^2} + \langle \hat{u} \rangle \hat{\zeta}_1 \frac{\partial \hat{C}^{(0)}}{\partial x} + \langle \hat{u} \rangle \hat{\zeta}_2 \frac{\partial \hat{C}^{(0)}}{\partial x} + \langle \hat{u} \rangle \hat{\zeta}_3 \frac{\partial \hat{C}^{(0)}}{\partial x} + k_s \hat{\chi}_1 \hat{C}^{(0)} + k_s \hat{\chi}_2 \hat{C}^{(0)} + k_s \hat{\chi}_3 \hat{C}^{(0)} = 0, \quad (4)$$

$$1 \left[ \frac{D}{R} + \hat{D}_{T_s} \frac{U^2 h^2}{D} + \hat{D}_{T_w} \frac{U^2 h^2}{D} \right] \frac{\partial^2 \hat{C}^{(0)}}{\partial x^2} + \langle \hat{u} \rangle \hat{\zeta}_1 \frac{\partial \hat{C}^{(0)}}{\partial x} + \langle \hat{u} \rangle \hat{\zeta}_2 \frac{\partial \hat{C}^{(0)}}{\partial x} + \langle \hat{u} \rangle \hat{\zeta}_3 \frac{\partial \hat{C}^{(0)}}{\partial x} + k_s \hat{\chi}_1 \hat{C}^{(0)} + k_s \hat{\chi}_2 \hat{C}^{(0)} + k_s \hat{\chi}_3 \hat{C}^{(0)} = 0, \quad (4)$$
where \( \hat{D}_{T_s} \) and \( \hat{D}_{T_w} \) are respectively the dispersion coefficients due to the steady and oscillatory flows and \( R = 1 + \hat{\alpha}_1 + \hat{\alpha}_2 \). The overbar denotes time average and angle brackets denote section average. The terms \( \hat{\zeta}_i \)’s and \( \hat{\chi}_i \)’s \((i = 1, 2, 3)\) are the effective coefficients for the advection and reaction respectively. Analytical expressions for the dispersion coefficients for the steady and oscillatory flows \( i.e. \hat{D}_{T_s} \) and \( \hat{D}_{T_w} \) have been derived but are not given here. Graphical variations for \( \hat{D}_{T_w} \) can be seen from figure (1).

Analytical expressions for all the advection and reaction coefficients can be obtained as

\[
\hat{\zeta}_1 = -\frac{\hat{\lambda}D_{a_s}}{6R^3}\left[5\hat{\alpha}_1^2 + 3\hat{\alpha}_2^2 - 4\hat{\alpha}_1\hat{\alpha}_2 + \hat{\alpha}_1 - \hat{\alpha}_2 + 12\left(\frac{\hat{\alpha}_1}{D_{a_1}} + \frac{\hat{\alpha}_2}{D_{a_2}}\right)\right],
\]

\[
\hat{\zeta}_2 = \frac{1}{R^2}\left[\hat{\lambda}^2\hat{\alpha}_1^m + \hat{\lambda}\hat{\alpha}_2^m\right], \quad \hat{\zeta}_3 = \frac{1}{R},
\]

\[
\hat{\chi}_1 = -\frac{n\hat{\lambda}^2D_{a_s}}{3R^5}\left[\hat{\alpha}_2^2 + \hat{\alpha}_1^2 - \hat{\alpha}_1\hat{\alpha}_2 + 3\left(\frac{\hat{\alpha}_1}{D_{a_1}} + \frac{\hat{\alpha}_2}{D_{a_2}}\right)\right],
\]

\[
\hat{\chi}_2 = \frac{m\hat{\lambda}}{R^2}\left[\hat{\lambda}^2\hat{\alpha}_1^m + \hat{\lambda}\hat{\alpha}_2^m\right], \quad \hat{\chi}_3 = \frac{\hat{\lambda}}{R}.
\]

Here in the expression of \( \hat{\zeta}_1 \) and \( \hat{\chi}_1 \), one has to take \( D_{a_s} = D_{a_1} \) for Case 1, \( D_{a_s} = D_{a_2} \) for Case 2 and without loss of generality, it is assumed that \( D_{a_s} = D_{a_1} = D_{a_2} \) for Case 3.

If there is no nonlinear reaction in the bulk flow and in the boundary, the chemical undergoes only reversible phase exchange with the flowing fluid \( i.e. \hat{\lambda} = \hat{\lambda}_s = \hat{\lambda}_d = 0 \).

So, the equation (4) is reduced to

\[
\frac{\partial \hat{C}^{(0)}}{\partial t} - \left[\frac{D}{R} + \hat{D}_{T_s} \frac{U^2h^2}{D} + \hat{D}_{T_w} \frac{U^2h^2}{D}\right] \frac{\partial^2 \hat{C}^{(0)}}{\partial x^2} + \langle \hat{u} \rangle \hat{\zeta}_3 \frac{\partial \hat{C}^{(0)}}{\partial x} = 0,
\]

and this equation coincides with the one obtained by Ng and Bai [4] in their work. This shows that, in the absence of nonlinearity the results are in good agreement with the existing literature.

5. Results and discussions

In this problem, effects of different parameters and chemical reaction on some transport coefficients have been studied.

The influence of \( \hat{D}_{T_w} \) with \( \hat{\delta} \) is shown in figure (1), where \( \hat{\delta} \) is the oscillation parameter. The value of \( \hat{\delta} \) will be smaller for higher angular frequency. The dispersion coefficient \( \hat{D}_{T_w} \) increases monotonically with \( \hat{\delta} \) for all sorbing cases. In other words, for a lower frequency the dispersion coefficient value will be higher. The enhancement effect gradually decreases as \( \hat{\delta} \) increases and beyond unity no remarkable effect on \( \hat{D}_{T_w} \) is observed. Again, among all three sorbing cases, Case 1 gives largest dispersion coefficient and Case 3 gives the least. Also, when both boundaries are inert, \( \hat{D}_{T_w} \) does not change in the plotted range of \( \hat{\delta} \).

Graphs of the reaction and advection coefficients \( \hat{\chi}_1 \) and \( \hat{\zeta}_1 \) against \( \hat{\alpha}_1 \) and \( \hat{\alpha}_2 \) are shown in figures (2a) and (2b) respectively for different degrees of nonlinearity. For a fixed value of \( n \), initially the graph of \( \hat{\chi}_1 \) decreases sharply to a minimum with increase of \( \hat{\alpha}_1 \) and \( \hat{\alpha}_2 \) and then it asymptotically approaches to zero. Large degree of nonlinearity for the decay reaction in the bulk flow reduces the value of the coefficient \( \hat{\chi}_1 \). Figure also shows that advection coefficient \( \hat{\zeta}_2 \) increases for \( m > 2 \) and remain stationary for \( m \leq 2 \) as \( \hat{\alpha}_1 \) and \( \hat{\alpha}_2 \) increase. Large degree of nonlinearity for the decay reaction at the boundaries shows the large value of the coefficient \( \hat{\zeta}_2 \).

The variations of transport coefficients \( \hat{\chi}_1 \) and \( \hat{\zeta}_1 \) with \( \hat{\lambda} \) can be seen from figure (3) for different values of retention parameters \( \hat{\alpha}_1 \) and \( \hat{\alpha}_2 \). It is clear from the figure that the coefficients \( \hat{\chi}_1 \) and \( \hat{\zeta}_1 \) are found to decrease. The changes are more noticeable for \( \hat{\chi}_1 \) than those for \( \hat{\zeta}_1 \) and the trends are undisturbed by any variations in \( \hat{\alpha}_1 \) and \( \hat{\alpha}_2 \).
Figure (4) shows the behavior of the advection coefficient $\hat{\zeta}_2$. It is seen from the figure that for all values of $\hat{\alpha}_1$ and $\hat{\alpha}_2$, $\hat{\zeta}_2$ increases with the increase of $\hat{\lambda}_s$ and $\hat{\lambda}_{s2}$, moreover, larger $\hat{\alpha}_1$ and $\hat{\alpha}_2$ increase the rate of enhancement of $\hat{\zeta}_2$.

![Figure 1](image1.png)

**Figure 1.** Variations of oscillatory dispersion coefficient $\hat{D}_{Tw}$ with oscillation parameter $\hat{\delta}$, where $\phi = 1.0$, $Sc = 0.1$ and $Da_1 = Da_2 = 1.0$.

![Figure 2](image2.png)

**Figure 2.** The transport coefficients $\hat{\chi}_1, \hat{\zeta}_2$ as a function of $\hat{\alpha}$ for different degrees of nonlinearity.
\[ \hat{\chi}_1, \hat{\zeta}_1, \hat{\lambda}, \hat{\alpha}_1 = \hat{\alpha}_2 = 0 \]

\[ n = 2, D_{a1} = D_{a2} = 1 \]

Figure 3. The transport coefficients \( \hat{\chi}_1, \hat{\zeta}_1 \) as a function of \( \hat{\lambda} \) for different values of \( \hat{\alpha} \).

Figure 4. The advection coefficient \( \hat{\zeta}_2 \) as a function of \( \hat{\lambda}_s \) for different values of \( \hat{\alpha} \).

6. Conclusions

Effects of different parameters and nonlinear reactions both within the bulk flow and at the wall on some transport coefficients are accounted explicitly. Some important conclusions are

(i) Lower angular frequency will give larger dispersion coefficients and coefficient is highly influence by wall sorption than inert boundary walls.

(ii) If the nonlinearity of the mobile phase reaction increases then its corresponding coefficient decreases whereas trend is opposite for the immobile phase reaction.

(iii) If the decay reaction rate in the bulk flow increases then corresponding coefficient decreases while result is opposite for decay reaction at the boundaries.

References

[1] Bandyopadhyay S and Mazumder BS 1999 *Int. J. Eng. Sci.* 37 1407
[2] Mei CC, Auriault JL and Ng CO 1996 *Adv. Appl. Mech.* 32 278
[3] Ng CO 2006 *Proc. R. Soc. A* 462 481
[4] Ng CO and Bai YC 2005 *Acta. Mech.* 178 65
[5] Paul S and Mazumder BS 2008 *Int. J. Eng. Sci.* 46 1203
[6] Paul S and Mazumder BS 2011 *Int. J. Heat Mass Tran.* 54 75
[7] Revelli R and Ridolfi L 2002 *J. Fluid Mech.* 472 307
[8] Revelli R and Ridolfi L 2003 *Adv. Water Resour.* 26 815
[9] Taylor GI 1953 *Proc. R. Soc. A* 219 186