

Laminar Dispersion in Presence of Slip and Chemical Reactions

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Abstract. Concentration profiles of a solute convectively diffusing and simultaneously undergoing homogeneous and heterogeneous chemical reactions under isothermal conditions in a non-Poiseuille laminar slip flow taking place in a closed parallel-plate channel with a permeable bed are presented. It is shown that presence of slip brings about an increase in concentration across the entire cross-section of the channel. Effect of varying reaction rate parameters on concentration profiles is also discussed.

1. Introduction

The dispersion of a substance dissolved in, or mixed with, a fluid flowing through channels has been the subject of study in a large number of analytic, numerical and experimental investigations. Among the notable contributions in the area are the works of Taylor^{1,2}, Aris³⁻⁵, Ananthakrishnan et al⁶, Gill and collaborators⁷. Shankarasubramanian and Gill⁸, Anderson and Berglin⁹, and Chatwin and Sullivan¹⁰. In all these investigations, it is assumed that the solute does not chemically react with the liquid in which it is dispersed. However, in a wide variety of problems of chemical engineering, diffusion of a solute takes place with simultaneous chemical reaction, e. g. hydrolysis of ester, gas absorption in an agitated tank with chemical reaction and so on¹¹. The problem of homogeneous and heterogeneous reactions in tubular flow reactors is of importance in several contexts. Situations of this type arise in gaseous phase homogeneous reactions where the tube walls have a catalytic effect. In the case of polymerisation reactions, the initiation may often be catalysed at the tube wall. Several interesting problems may be formulated so that the governing equations with relevant boundary conditions correspond to the problem of simultaneous homogeneous and heterogeneous reactions in tubular flow. An example of this may be the flow of a nuclear fuel through a channel where heat is generated in the bulk (analogous to a homogeneous reactor source)

and heat is removed at the walls under constant heat flux conditions (analogous to a zero order heterogeneous reaction) or under finite surface resistance conditions (analogous to a first order catalytic reaction).

There are several analytical and numerical investigations concerned with tube flow in the presence of homogeneous and heterogeneous chemical reactions under different sets of boundary conditions. Bauer¹² has studied this problem of dispersion of a solute in laminar flow between two parallel plates. In all these papers, the basic flow satisfied no-slip condition at the channel walls. The main objective of this paper is to study the effect of tangential velocity slip on concentration profiles of a solute convectively diffusing and simultaneously undergoing homogeneous reaction in the bulk of the fluid and heterogeneous reaction at the catalytic wall, for laminar flow through a parallel-plate channel with a permeable bed. The resulting eigen boundary value problem is solved analytically to yield a solution for concentration distribution in the form of an eigenfunction expansion involving confluent hypergeometric functions. Effect of varying reaction rate parameters on concentration profiles is clearly brought out in this paper for the cases of slip and no-slip boundary conditions satisfied by the basic flow at the lower boundary of the channel.

2. Basic flow field

We consider laminar flow of an incompressible viscous fluid in a closed parallel-plate channel whose bed is permeable and the upper boundary is an impermeable plane at distance $2h$ from the bed. The flow within the porous material of the bed occupying the region $y < -h$ and the flow in the free-flow region $-h < y < h$ are both assumed to be generated and maintained by a uniform axial pressure gradient. We choose a frame of reference having origin midway between the plane boundaries, the positive x -axis along the direction of flow and y -axis vertically upwards with the boundaries situated at $y = \pm h$. A velocity field of the form $(u(y), 0, 0)$ satisfies the equation of continuity.

$$\frac{\partial u}{\partial x} = 0 \quad (1)$$

The uniform Darcy velocity Q of the flow within the porous material of the bed ($y < -h$) is given by

$$Q = -\frac{k}{\mu} \frac{dp}{dx} \quad (2)$$

where k (cm^2), μ and p respectively denote the permeability of the porous medium, dynamic viscosity of the fluid and flow pressure distribution.

The momentum equation for flow in the region $-h < y < h$, is

$$\frac{d^2u}{dy^2} = \frac{1}{\mu} \frac{dp}{dx} \quad (3)$$

and the relevant boundary conditions to be satisfied by $u(y)$ are:

(i) slip condition at the lower permeable boundary¹³.

$$\frac{du}{dy} = \frac{\alpha}{\sqrt{k}}(U - Q) \text{ at } y = -h \quad (4a)$$

and

(ii) no-slip condition at the upper boundary

$$u = 0 \text{ at } y = h \quad (4b)$$

in which α is a dimensionless constant depending on the structure of the porous material and $U = \lim_{y \rightarrow -h} u(y)$ denotes slip velocity at the interface $y = -h$. We shall be determining U as part of the solution.

Introducing the dimensionless normal distance coordinate $\eta = y/h$, the velocity profile in the parallel-plate channel obtained on solving Eqn. (3) subject to boundary conditions (4), is

$$u(\eta) = \frac{1}{2} [(1 - \eta)U + (1 - \eta^2)V] \quad (5)$$

with the slip velocity U given by

$$U = \frac{2(\alpha + \sigma)}{\sigma(1 + 2\alpha\sigma)} V \quad (9)$$

in which we have introduced the dimensionless permeability parameter $\sigma = h/\sqrt{k}$ and the constant $V = -h^2/\mu \frac{dp}{dx}$ which has the dimensions of velocity and is known from the prescribed experimental conditions.

3. Convective-Diffusion with Slip and Simultaneous Homogeneous and Heterogeneous Chemical Reactions

Now, we consider a solute which convectively diffuses in the fully-developed flow described by Eqns. (5) & (6) and which also simultaneously undergoes a first order homogeneous reaction in the bulk of the fluid with rate constant K_1 and a heterogeneous reaction at the boundaries which are assumed to be catalytic. Under isothermal conditions, the local concentration $c(x, y)$ of solute satisfies the equation

$$u(\eta) \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial y^2} - K_1 c \quad (7)$$

where D is the molecular diffusion coefficient assumed to be constant. In writing eqn. (7), longitudinal diffusion is neglected in comparison to transverse diffusion.

The appropriate boundary conditions for $c(x, y)$ are

$$\begin{aligned} \frac{\partial c}{\partial y} &= -f_1 c \text{ at } y = h \\ \frac{\partial c}{\partial y} &= f_2 c \text{ at } y = -h \end{aligned} \quad (8)$$

where f_1, f_2 denote heterogeneous reaction rate constants corresponding to catalytic reaction at the upper and lower boundaries respectively.

Introducing the dimensionless axial distance coordinate $\xi = x/h$ and seeking a solution of the form

$$c(\xi, \eta) = \bar{c}(\eta)e^{-\lambda \xi} \quad (9)$$

Eqns. (7) and (8) then give

$$\frac{d^2 \bar{c}}{d\eta^2} + (\lambda \omega(\eta) - \delta^2) \bar{c} = 0 \quad (10)$$

with $\bar{c}(\eta)$ satisfying the boundary conditions

$$\begin{aligned} \frac{d\bar{c}}{d\eta} &= -\beta_1 \bar{c} \text{ at } \eta = 1 \\ \frac{d\bar{c}}{d\eta} &= \beta_2 \bar{c} \text{ at } \eta = -1 \end{aligned} \quad (11)$$

where

$$\omega(\eta) = \frac{P_e}{2} [(1 - \eta) \frac{U}{V} + (1 - \eta^2)], \text{ with } \frac{U}{V} \text{ known from Eqn. (6)}$$

$$P_e = \frac{hV}{D} \text{ is Peclet number}$$

$$\delta = h \sqrt{\frac{K_1}{D}} \text{ is dimensionless homogeneous reaction rate parameter}$$

and

$$\beta_1 = f_1 h, \beta_2 = f_2 h \text{ are dimensionless heterogeneous reaction rate parameters.}$$

Eqns. (10) and 11 comprise a Sturm-Liouville eigen boundary value problem with λ as eigen parameter and $\omega(\eta)$ as the weight function. Since $\omega(\eta) \geq 0$ in $-1 \leq \eta \leq 1$ (ω vanishes only at $\eta = 1$), all the eigenvalues λ are real and positive. Note that $\lambda = 0$ is an eigenvalue in the case only when $\delta = 0$ and $\beta_1 = \beta_2 = 0$ (i.e. absence of chemical reactions). Thus the boundedness of the solution of the form assumed in Eqn. (9) is ensured ($\xi > 0$). A few general inferences concerning the

behaviour of λ with variation in the parameters δ and β_1, β_2 can be made from the theory of Sturm-Liouville problems¹⁴. If β (β_1 or β_2) is increased monotonically from zero to infinity, each eigenvalue will increase monotonically from its value for $\beta = 0$ to its value for $\beta = \infty$. Furthermore the difference $\lambda_{n+1} - \lambda_n$ becomes independent of β for sufficiently large n . The behaviour with variation in δ is similar in that each λ increases monotonically with monotonically increasing δ . Computed values of λ presented in Tables 1-3 support the observations made above.

Since all the eigenvalues λ_n of the problem described by Eqns. (10) and (11) are non-negative, we find it convenient to introduce a new eigen parameter Λ which is related to λ through the relation

$$\Lambda^2 = \frac{\lambda P_e}{2}$$

Then the eigenvalues $\Lambda_n, n = 1, 2, \dots$ of this problem are given by the roots of the transcendental equation (Appendix)

$$PM - TN = 0 \tag{12}$$

Table 1. Eigenvalues λ_n for different values of homogeneous and heterogeneous reaction rate parameters (β_1, β_2) ($U/V = 0.005386, P_e = 25$).

n/β_2	$\beta_1 = 0$			$\beta_1 = 4$			$\beta_1 = 8$			
	0	4	8	0	4	8	0	4	8	
1	1.56	1.60	1.61	1.61	1.62	1.63	1.60	1.62	1.63	$\delta = 4$
2	2.38	2.47	2.49	2.46	2.56	2.58	2.48	2.59	2.61	
3	3.48	3.66	3.70	3.66	3.84	3.90	3.70	3.90	3.94	
4	4.92	5.16	5.22	5.18	5.42	5.48	5.22	5.48	5.54	
5	6.58	6.84	6.92	6.84	7.10	7.17	6.92	7.16	7.24	
6	8.28	8.50	8.58	8.50	8.76	8.84	8.56	8.84	8.93	
7	9.18	9.33	9.40	9.34	9.42	9.48	9.42	9.48	9.52	
8	13.18	13.38	13.58	13.16	14.40	14.67	13.17	14.40	14.99	
9	13.40	14.40	14.98	14.66	14.68	14.98	15.28	15.29	15.30	
1	5.74	5.74	5.76	5.74	5.75	5.76	5.75	5.76	5.77	$\delta = 8$
2	7.22	7.23	7.23	7.24	7.26	7.26	7.24	7.26	7.27	
3	8.88	8.92	8.93	8.92	8.95	8.97	8.92	8.96	8.99	
4	10.58	10.66	10.67	10.65	10.73	10.74	10.66	10.74	10.76	
5	12.04	12.12	12.14	12.12	12.20	12.21	12.15	12.20	12.23	
6	14.12	14.27	14.26	14.16	14.48	14.56	14.16	14.49	14.59	
7	14.36	14.56	14.62	14.66	14.69	14.70	14.76	14.77	14.78	
8	20.17	22.10	22.12	21.66	23.52	22.04	21.66	23.52	24.30	
9	22.10	23.52	24.30	24.04	24.08	24.30	24.82	24.83	24.85	

Table 2. Eigenvalues λ_n for different values of homogeneous and heterogeneous reaction rate parameters in the case of absence of slip ($U/V = 0, P_0 = 25$)

n/β_2	$\beta_1 = 0$			$\beta_1 = 4$			$\beta_1 = 8$		
	0	4	8	0	5	8	0	4	8
1	1.59	1.60	1.61	1.60	1.62	1.63	1.61	1.63	1.64
2	2.40	2.48	2.50	2.48	2.59	2.61	2.50	2.61	2.63
3	3.51	3.68	3.73	3.68	3.88	3.92	3.72	3.93	3.97
4	4.97	5.20	5.26	5.20	5.46	5.52	5.27	5.52	5.58
5	6.64	6.90	6.96	6.90	7.14	7.22	6.96	7.22	7.29
6	8.34	8.58	8.64	8.58	8.84	8.92	8.64	8.92	9.01
7	9.24	9.40	9.48	9.40	9.50	9.54	9.48	9.54	9.59
8	13.42	13.48	13.54	13.42	14.72	14.72	13.42	14.72	15.32
9	13.44	14.72	15.32	14.72	14.76	15.32	15.32	15.34	15.38
$\delta = 4$									
1	5.76	5.78	5.79	5.78	5.79	5.80	5.78	5.79	5.81
2	7.28	7.29	7.30	7.38	7.31	7.32	7.33	7.33	7.36
3	8.94	8.98	8.99	8.98	9.01	9.03	8.98	9.02	9.04
4	10.66	10.73	10.75	10.72	10.80	10.83	10.75	10.82	10.84
5	12.14	12.20	12.23	12.21	12.28	12.30	12.22	12.29	12.31
6	14.25	14.34	14.35	14.31	14.56	14.66	14.34	14.66	14.72
7	14.44	14.72	14.80	14.72	14.77	14.83	14.81	14.83	14.87
8	22.16	22.19	22.24	22.17	24.10	24.12	22.16	24.11	24.91
9	22.36	24.10	24.90	24.10	24.12	24.16	24.90	24.94	24.96
$\delta = 8$									

Table 3. Eigenvalues λ_n in the case of absence of homogeneous and heterogeneous reactions.

$\delta = 0, \beta_1, \beta_2 = 0$		
n	$U/V = 0.005386$	$U/V = 0$
	$(\alpha = 4.0, \sigma = 50)$	
1	0.00	0.00
2	0.41	0.42
3	1.43	1.45
4	2.91	2.94
5	4.06	4.71
6	6.44	6.48
7	7.62	7.67
8	10.70	10.88
9	10.87	10.92

where

$$P = 4 l \Lambda Q_1 {}_1F_1 \left(l + 1, \frac{3}{2}; \Lambda Q_1^2 \right) + (\beta_1 - \Lambda Q_1) {}_1F_1 \left(l, \frac{1}{2}; \Lambda Q_1^2 \right)$$

$$T = (1 + \beta_1 Q_1 - \Lambda Q_1^2) {}_1F_1 \left(l + \frac{1}{2}, \frac{3}{2}; \Lambda Q_1^2 \right)$$

$$+ \frac{2}{3} (2l + 1) \Lambda Q_1^2 {}_1F_1 \left(l + \frac{3}{2}, \frac{5}{2}; \Lambda Q_1^2 \right)$$

$$M = 4l \Lambda Q_2 {}_1F_1 \left(l + 1, \frac{3}{2}; \Lambda Q_2^2 \right) - (\beta_2 + \Lambda Q_2) {}_1F_1 \left(l, \frac{1}{2}; \Lambda Q_2^2 \right)$$

$$N = (1 - \beta_2 Q_2 - \Lambda Q_2^2) {}_1F_1 \left(l + \frac{1}{2}, \frac{3}{2}; \Lambda Q_2^2 \right)$$

$$+ \frac{2}{3} (2l + 1) \Lambda Q_2^2 {}_1F_1 \left(l + \frac{3}{2}, \frac{5}{2}; \Lambda Q_2^2 \right)$$

in which

$$l = \frac{\delta^2 + \Lambda - \left(\frac{U}{2V} + 1 \right)^2 \Lambda^2}{4\Lambda}$$

$$Q_1 = \frac{U}{2V} + 1, \quad Q_2 = \frac{U}{2V} - 1$$

and ${}_1F_1(a, b; x)$ represents confluent hypergeometric function.

The eigenfunctions $\bar{c}_n(\eta)$ corresponding to the eigen values $\Lambda_n, n = 1, 2, \dots$ are given by

$$\begin{aligned} \bar{c}_n(\eta) = e^{-Y_n/\Lambda_n} & \left[{}_1F_1 \left\{ \frac{1}{4\Lambda_n} \left(\delta^2 + \Lambda_n - \left(1 + \frac{U}{2V} \right)^2 \Lambda_n^2 \right), \frac{1}{2}; Y_n \right\} \right. \\ & \left. - \frac{P_n}{T_n} \sqrt{Y_n} {}_1F_1 \left\{ \frac{1}{4\Lambda_n} \left(\delta^2 + 3\Lambda_n - \left(1 + \frac{U}{2V} \right)^2 \Lambda_n^2 \right), \frac{3}{2}; Y_n \right\} \right], \\ n = 1, 2, \dots \end{aligned} \tag{13}$$

where $Y_n = \left(\eta + \frac{U}{2V} \right)^2 \Lambda_n$ and P_n, T_n designate the expressions for P and T evaluated at $\Lambda = \Lambda_n, n = 1, 2, \dots$

The concentration $c(\xi, \eta)$ is then obtained from

$$c(\xi, \eta) = \sum_{n=1}^{\infty} A_n c_n(\eta) e^{-\Lambda_n \xi} \tag{14}$$

in which the constants A_n on using the orthogonality relation

$$\int_{-1}^1 \omega(\eta) \bar{c}_m(\eta) \bar{c}_n(\eta) d\eta = 0, m \neq n \quad (15)$$

and the inlet condition, say

$$c(0, \eta) = 1 \quad (16)$$

come out to be

$$A_n = \frac{\int_{-1}^1 \omega(\eta) \bar{c}_n(\eta) d\eta}{\int_{-1}^1 \omega(\eta) \bar{c}_n^2(\eta) d\eta} \quad n = 1, 2, \dots$$

4. Results and Discussion

For the purpose of computations, we have taken $\alpha = 4$, $\sigma = 50$. These values of α , σ give (from Eqn. (6)) $U/V = 0.53865 \times 10^{-2}$. The first nine eigenvalues for several values of homogeneous (δ) and heterogeneous (β) reaction rate parameters in the presence ($U/V \neq 0$) and absence ($U/V = 0$) of slip are presented in Tables 1-3. As expected, we note that the eigenvalues increase monotonically with increase in the values of δ and β . It is also observed that the eigenvalues have lower value in the presence of slip than in the case of no-slip.

The concentration profiles at the axial location $\xi = 1$ for $\delta = 4, 8$ and $\beta_1 = \beta_2 = 0, 4, 12$ are shown in Figs. 1 and 2. The solid and dotted curves correspond to the presence and absence of slip respectively. We note that for the entire range

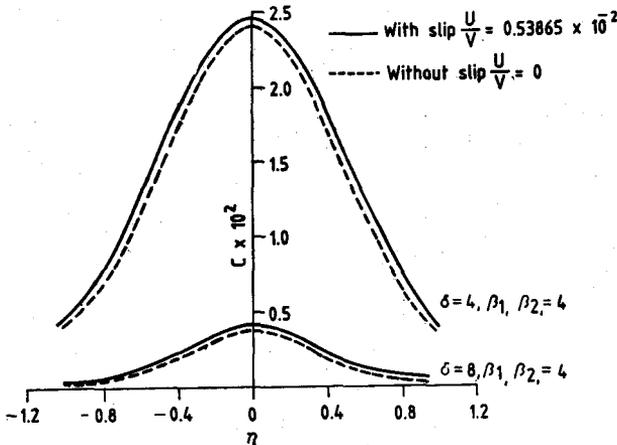


Figure 1. Representative concentration profiles for different values of β and δ at $\xi = 1$.

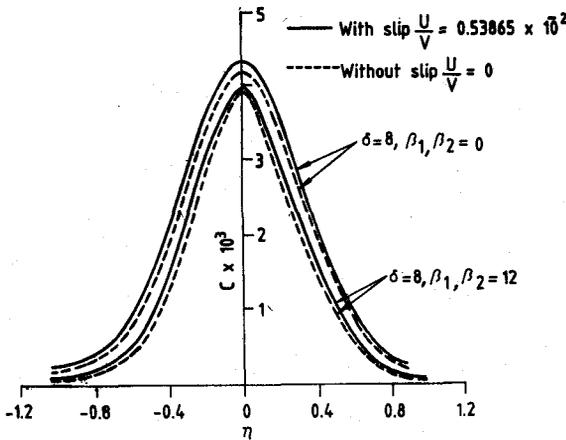


Figure 2. Representative concentration profiles for different values of δ and β at $\xi = 1$.

of values of δ and β , the concentration increases on account of slip at every point in the channel cross-section. Furthermore, when one of the two parameters δ and β is held fixed, an increase in the other causes a decrease in the distribution of concentration. This result holds in the presence as well as absence of slip.

References

1. Taylor, G. I., *Proc. Roy. Soc. Lond.*, **A219** (1953), 186.
2. Taylor, G. I., *Proc. Roy. Soc. Lond.*, **A223** (1954), 476.
3. Aris, R., *Proc. Roy. Soc. Lond.*, **A235** (1956), 67.
4. Aris, R., *Proc. Roy. Soc. Lond.*, **A252** (1959), 538.
5. Aris, R., *Proc. Roy. Soc. Lond.*, **A259** (1960), 370.
6. Ananthkrishnan, V., Gill, W. N. & Barduhn, A. J., *A. I. Ch. E. J.*, **11** (1965), 1063.
7. Gill, W. N., Ananthkrishnan, V. & Nunge, R. J., *A. I. Ch. E. J.*, **14** (1968), 939.
8. Shankarasubramanian, R. & Gill, W. N., *Proc. Roy. Soc. Lond.*, **A333** (1973), 115.
9. Anderson, B. & Berglin, T., *Proc. Roy. Soc. Lond.*, **A377** (1981), 251.
10. Chatwin, P. C. & Sullivan, P. J., *J. Fluid Mech.*, **120** (1982), 347.
11. Bird, R. B., Stewart, W. E. & Lightfoot, E. N., 'Transport Phenomena' (Wiley, New York), 1960.
12. Bauer, H. F., *Int. J. Heat Mass Transfer*, **19** (1976), 479.
13. Beavers, G. S. & Joseph, D. D., *J. Fluid Mech.*, **30** (1967), 197.
14. Birkoff, G. & Rota, G. C., 'Ordinary Differential Equations' (Wiley, New York), 1978.
15. Slater, L. J., 'Confluent Hypergeometric Functions' (Cambridge University Press), 1960.

Appendix

Derivation of Equation giving Eigenvalues

On introducing the transformations

$$Y = \left(\eta + \frac{U}{2V} \right)^2 \Delta, \quad c^-(\eta) v(Y) e^{-Y/2} \quad (i)$$

the Eqn. (10) becomes

$$Yv'' + \left(\frac{1}{2} - Y \right) v' - \frac{1}{4\Lambda} \left(\delta^2 + \Lambda - Q_1^2 \Lambda^2 \right) v = 0 \quad (\text{ii})$$

wher $\Lambda^2 + \frac{\lambda P_e}{2}$, $Q_1 = 1 + \frac{U}{2V}$ and prime denotes derivative with respect to Y .

The homogeneous differential Eqn. (ii) is the confluent hypergeometric equation (Kummer's equation) whose solution is given in Slater¹⁵.

$$v(Y) = A {}_1F_1 \left(\frac{\delta^2 + \Lambda - Q_1^2 \Lambda^2}{4\Lambda}, \frac{1}{2}; Y \right) + B {}_1F_1 \left(\frac{\delta^2 + 3\Lambda - Q_1^2 \Lambda^2}{4\Lambda}, \frac{3}{2}; Y \right) \sqrt{Y} \quad (\text{iii})$$

For non-trivial solutions to exist, use of boundary conditions (11) then yields Eqn. (12) whose roots give the eigenvalues of the problem studied in this paper.