

Dispersion in Presence of Slip and Chemical Reactions in Porous-Wall Tube Flow

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ABSTRACT

This paper deals with the problem of studying the effect of tangential velocity slip on the concentration profiles of a solute which is convectively diffusing and simultaneously undergoing irreversible, first order homogeneous and heterogeneous chemical reactions in a porous wall tube, under isothermal laminar flow conditions. It is shown that the presence of velocity slip at the porous wall induces an increase in the concentration of solute across the entire cross-section of the tube while an increase in the rates of chemical reactions is found to reduce the concentration under both slip and no-slip boundary conditions. Accurate eigenvalues, eigenfunctions and the concentration profiles are determined for the cases when slip or no-slip boundary condition holds at the wall.

1. INTRODUCTION

The problem of dispersion in the presence of simultaneous homogeneous and heterogeneous chemical reactions is of importance in several contexts, for example, in technical and nuclear physics, gas absorption in an agitated tank, biological systems and the flow of a nuclear fuel in a tube where heat is generated in the bulk (analogous to homogeneous reaction in the bulk of the fluid) and when heat is removed at the wall under constant heat flux condition (zero order heterogeneous reaction at the wall) or under finite surface resistance condition which corresponds to a first order heterogeneous catalytic reaction at the wall¹. Situations of this type also arise in gaseous phase homogeneous reactions when the tube wall has a catalytic effect, implying heterogeneous reaction at the wall. The wide variety of these interesting problems lead to a formulation in which the governing equations together with the

relevant boundary conditions are similar to those for the problem of dispersion in tubular flow reactors when homogeneous and heterogeneous reactions are occurring simultaneously.

There are numerous analytical and numerical investigations dealing with tube flow in presence of either or both homogeneous and heterogeneous chemical reactions. The survey of literature pertinent to flow problems with chemical reactions reveals that Cleland and Wilhelm² considered the case of no heterogeneous reaction with finite difference method and supported their theoretical profiles with experimental data. Sellars³ *et al* studied asymptotically the classical Graetz problem, namely no homogeneous reaction and infinite heterogeneous reaction. Katz⁴ considered heterogeneous reactions from an integral equation view point. Hsu⁵ solved the problem of finite first order homogeneous reaction but no heterogeneous reaction by numerical integration for one value of homogeneous reaction rate constant. Work on combined first order homogeneous and heterogeneous reactions has been reported by Walker⁶ who considered both radial and axial diffusion but reported only the first eigenvalue and studied the concentration profiles from an asymptotic view point. Krongelb and Strandberg⁷ used finite difference method to investigate second order homogeneous reactions with first order heterogeneous kinetics. Solomon and Hudson⁸, employing Galerkin method, analysed the tube flow problem to deduce the criteria under which homogeneous reactions may be neglected with respect to heterogeneous reactions and vice versa. Bauer^{9,10} presented solutions in eigenfunction expansions involving confluent hypergeometric series for parallel-plate and cylindrical tube flow problems when the basic flow satisfied no slip boundary condition at the impermeable wall and the concentration satisfied different boundary conditions, namely, constant wall concentration, constant concentration flux and first order heterogeneous reaction at the wall.

In all these investigations the wall of the channel were taken to be impermeable and hence no-slip condition was used to determine the basic flow for which the dispersion problem is studied. When the tube wall is made up of a porous material, an appropriate slip boundary condition proposed by Beavers and Joseph¹¹ replaces the no-slip condition for the impermeable wall. In this paper, we study the combined effect of tangential velocity slip and homogeneous and heterogeneous chemical reactions on the concentration profiles of a solute in a dilute system under isothermal laminar flow conditions. Bauer^{9,10} studied the problem in the absence of slip at the boundary. The results reported by Solomon and Hudson⁸ and Bauer¹⁰ follow as a special limiting case of the present study. Laminar dispersion in presence of slip and chemical reactions for parallel-plate channel flow has been investigated and reported in our earlier paper¹².

2. BASIC VELOCITY FIELD

We obtain the velocity profiles of the axi-symmetric laminar flow of an incompressible viscous fluid in a circular tube of radius a , when its wall is made up of a porous material of permeability k . The conventional approach to study such flows is to regard the flow domain to be divided into two parts, namely, the flow within

the porous material of the thick wall and the flow in the tube. Both these flows are generated and maintained by a uniform axial pressure gradient. We use cylindrical polar coordinates (r, θ, x) with the x -axis along the axis of the tube in the direction of flow; r, θ, x denote radial, azimuthal and axial coordinates of a point in the flow domain.

Let $u(r)$ denote the only non-zero axial component of fluid velocity. Then the velocity field $[0, 0, u(r)]$ is compatible with the equation of continuity

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

The uniform velocity Q of flow within the porous medium of the wall is given by Darcy law, namely

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

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

The momentum equation for the laminar flow in the region $0 < r < a$ for the problem under study simplifies to

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{du}{dr} \right) = \frac{1}{\mu} \frac{dp}{dx} \quad (3)$$

The relevant boundary conditions for u are

$$(i) \quad \frac{du}{dr} = 0 \quad \text{at} \quad r = 0 \quad (4a)$$

$$(ii) \quad \frac{du}{dr} = -\frac{a}{\sqrt{k}}(u - Q) \quad \text{at} \quad r = a \quad (4b)$$

where a is a dimensionless constant depending on the structure of the porous medium.

In the limiting case of $k \rightarrow 0$, it is readily seen that Eqn. (4b) reduces to the no-slip condition $u = 0$ at $r = a$

Introducing the following dimensionless quantities

$$\eta = \frac{r}{a}, \text{ normal distance coordinate}$$

$$a = \frac{b}{\sqrt{k}} \text{ permeability parameter}$$

and $u_c = -\frac{a^2}{\mu} \frac{dp}{dx}$, positive characteristic velocity, completely determined

from the prescribed flow conditions, the solution of Eqn. (3) satisfying the boundary conditions (4a, 4b) can be written as

$$u(\eta) = u_s + \frac{1}{4} (1-\eta^2) u_c \quad (5)$$

where

$$u_s = \frac{2a + \sigma}{2a\sigma^2} u_c \quad (6)$$

denotes the slip velocity at the inner permeable interface of the two flow regions. It can be easily verified from Eqn. (6) that in the limiting case of zero permeability, ie when $\sigma \rightarrow \infty$, the slip velocity u_s approaches the value zero, as expected.

3. CONVECTIVE-DIFFUSION WITH SIMULTANEOUS HOMOGENEOUS AND HETEROGENEOUS REACTIONS

We now consider a solute convectively diffusing in the basic flow field described by Eqns. (5) and (6) in the presence of simultaneous homogeneous and heterogeneous chemical reactions, under isothermal laminar conditions. The differential material balance of the solute at any point in the tube then gives the following equation for solute concentration $c(x, r)$,

$$u(\eta) \frac{\partial c}{\partial x} = D \left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} \right) - K_1 c \quad (7)$$

in which D is the coefficient of molecular diffusion, assumed constant and K_1 denotes the first order homogeneous reaction rate constant.

The term $-K_1 c$ in Eqn. (7) represents the volume rate of annihilation of solute due to chemical reaction in the bulk of the fluid. In writing Eqn. (7), we have assumed that (i) the solution is dilute so that the basic flow is not disturbed and (ii) $\frac{\partial^2 c}{\partial x^2} \ll \frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r}$ that is, the diffusion in the axial direction is negligible compared to the radial diffusion because axial dispersion is governed more by the mechanism of convection than molecular diffusion. Eqn. (7) will be solved subject to the following inlet condition and boundary conditions :

Inlet Condition :

$$c(x, r) = c_0, \text{ a constant at } x = 0, 0 < r < a \quad (8)$$

Boundary Conditions :

(i) on the catalytic tube wall :

$$\frac{\partial c}{\partial r} = -fc \text{ at } r = a, x > 0 \quad (8a)$$

(ii) a regularity condition on the axis of tube :

$$\frac{\partial c}{\partial r} = 0 \text{ at } r = 0, x > 0 \quad (8b)$$

In (8a), f (cm^{-1}) denotes the heterogeneous reaction rate constant corresponding to the catalytic reaction at the tube wall.

On introducing the dimensionless axial distance variable $\xi = \frac{x}{a}$ and dimensionless concentration $c' = \frac{c}{c_0}$, the above system of equations after dropping prime over c' can be written as

$$\frac{\partial^2 c}{\partial \eta^2} + \frac{1}{\eta} \frac{\partial^2 c}{\partial \eta} - \delta^2 c = \frac{P_e}{u_c} u(\eta) \frac{\partial c}{\partial \xi} \quad (9)$$

$$c(\xi, \eta) = 1 \quad \text{at } \xi = 0, 0 < \eta < 1 \quad (10)$$

$$\frac{\partial c}{\partial \eta} = -\beta c \quad \text{at } \eta = 1, \xi > 0 \quad (10a)$$

$$\frac{\partial c}{\partial \eta} = 0 \quad \text{at } \eta = 0, \xi > 0 \quad (10b)$$

in which $P_e = \frac{au_c}{D}$ is Peclet number and $\delta = a\sqrt{\frac{K_1}{D}}$, $\beta = fa$ are dimensionless homogeneous and heterogeneous reaction rate parameters respectively.

To solve the problem described by the system (9) – (10b), we assume a solution of the form

$$c(\xi, \eta) = \bar{c}(\eta)e^{-\lambda\xi} \quad (11)$$

in which λ is a positive-valued parameter.

On using Eqn. (11), Eqns. (9) and (10a,b) become

$$\frac{d}{d\eta} \left(\eta \frac{d\bar{c}}{d\eta} \right) + [\lambda\omega(\eta) - \delta^2\eta] \bar{c} = 0 \quad (12)$$

$$\frac{d\bar{c}}{d\eta} = -\beta\bar{c} \quad \text{at } \eta = 1, \xi > 0 \quad (13a)$$

$$\frac{d\bar{c}}{d\eta} = 0 \quad \text{at } \eta = 0, \xi > 0 \quad (13b)$$

where

$$\omega(\eta) = P_e \eta \left[\frac{u_s}{u_c} + \frac{1}{4}(1-\eta^2) \right] \quad (14)$$

Equations (12) and (13a,b) comprise a Sturm-Liouville eigen boundary value problem with $\omega(\eta)$ as the weight function and λ , an eigen parameter.

On introducing the quantities Y , f and A defined by

$$Y = A\eta^2, \quad f(Y) = \bar{c} e^{Y/2} \quad \text{and} \quad A^2 = \frac{\lambda P_e}{4} \quad (15)$$

we find that Eqn. (12) takes the form

$$Yf'' + (1-Y)f' - lf = 0 \quad (16)$$

in which prime denotes differentiation with respect to Y and l , which depends on A , δ and $\frac{u_s}{u_c}$, is given by

$$l = \frac{1}{4A} \left[\delta^2 + 2A - \left(1 + 4\frac{u_s}{u_c}\right)A^2 \right] \quad (17)$$

Equation (16) is the confluent hypergeometric differential equation. Its general solution can be written as

$$f(Y) = A_1 F_1(l, 1, Y) + B_1 F_1(l, 1, Y) \ln Y + \sum_{s=1}^{\infty} B_s Y^s \quad (18)$$

in which

$$B_s = \frac{\Gamma(l+s)}{(s!)^2} \sum_{m=0}^{s-1} \left(\frac{1}{l+m} - \frac{2}{m+1} \right)$$

A , B are arbitrary constant, $\Gamma(\cdot)$ denotes gamma function and ${}_1F_1(\dots)$ stands for confluent hypergeometric series. In order that the solution be bounded at $Y = 0$ (i.e. $\eta = 0$), the boundary condition (13b) demands that we take $B = 0$ in the solution (18). Then, on using the boundary condition (13a) and the result [ref 13, page 15, Slater (1960)]

$$\frac{d}{dx} [{}_1F_1(a, b, x)] = \frac{a}{b} {}_1F_1(a+1, b+1, x)$$

we find that Eqn. (16) can have a nontrivial solution only when A takes on the values A_n , $n = 1, 2, \dots$ which are roots of the equation

$$2Al {}_1F_1(l+1, 2, A) + (\beta-A) {}_1F_1(l, 1, A) = 0 \quad (19)$$

The eigenfunctions $\bar{C}_n(\eta)$ corresponding to the eigen values A_n , $n = 1, 2, 3, \dots$ are given by

$$\bar{C}_n(\eta) = e^{-A_n \eta} \frac{\eta^2}{2} {}_1F_1(l_n, 1, A_n \eta^2) \quad (20)$$

where l_n stands for the expression l when A is replaced by A_n

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

$$C(\xi, \eta) = \sum_{n=1}^{\infty} A_n \bar{C}_n(\eta) e^{-4A \frac{2}{n} \xi/P_c} \quad (21)$$

in which the constants A_n , on using the orthogonality condition

$$\int_0^1 \omega(\eta) \bar{C}_m(\eta) \bar{C}_n(\eta) d\eta = 0, \quad m \neq n \quad (22)$$

and the inlet condition

$$C(0, \eta) = 1$$

are computed from

$$A_n = \frac{\int_0^1 \omega(\eta) \bar{C}_n(\eta) d\eta}{\int_0^1 \omega(\eta) \bar{C}_n^2(\eta) d\eta}, \quad n = 1, 2, \dots \quad (23)$$

4. NUMERICAL DETAILS AND RESULTS

It is noticed from Eqn. (14), that the weight function $\omega(\eta)$ of the Sturm-Liouville Eqn. (12) is positive for $0 < \eta < 1$. It, therefore, follows that all the eigenvalues are real-valued and positive. A few general conclusions concerning the behaviour of λ with variation in β and δ can be made from the theory of S-L eigenvalue problems. If β 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 $\lambda_{n+1} - \lambda_n$ will be independent of β for sufficiently large n . The behaviour with δ is similar in that each λ increases monotonically with increasing δ .

Computations were done with double precision on an ICL 2960 computer, at the fixed axial location $\xi = 1$ for parameter values $a = 4$, $\sigma = 50$ and $P_e = 100$. The first nine roots of Eqn. (19) were determined by Newton-Raphson method for reaction rate parameters $\beta = 0, 4, 12$ and $\delta = 0, 4, 8$ for the cases of no-slip and finite tangential velocity slip at the boundary. For the particular porous material¹¹ considered in this study, the value of the dimensionless slip velocity $\frac{u_s}{u_c}$ came out to be 0.0029. Having found sufficiently accurate values of A_n , $n = 1, 2, \dots, 9$ from Eqn. (19), the corresponding eigenfunctions were then determined numerically from Eqn. (12) by finite differencing. The numerically evaluated eigenfunctions were in turn used in Eqn. (23) to evaluate the constants A_n . Since the exponential factor in successive terms of Eqn. (21) decreases with increasing A_n , the first nine terms of the series were found adequate to yield accurate concentration profiles. The results of the trial were checked against those with seven terms of the series and no significant change was observed in the computed values of concentration. Tables 1-3 display the first nine eigenvalues λ_n , $n = 1, 2, \dots, 9$ for different values of reaction rate parameters under slip and no-slip conditions. It is observed from these tables that the eigenvalues increase monotonically with increase in the homogeneous and heterogeneous reaction rate parameters. This is in accord with the prediction of S-L theory. Also, the presence of slip at the wall induces a decrease in the eigenvalues for all values of β and δ . In other words, for any fixed values of β and δ , the eigenvalues assume their maximum values when no-slip condition holds at the boundary, that is, when the tube wall is impermeable.

Table 1. First nine eigenvalues λ_n under slip condition when $P_e = 100$, $\frac{u_s}{u_c} = 0.0029$, $\alpha = 4$ and $\sigma = 50$.

$n \backslash \beta$	λ_n				
	0	4	8	12	
1	0.97	1.03	1.04	1.05	
2	2.17	2.46	2.54	2.57	
3	4.38	4.84	5.00	5.08	
4	7.53	8.01	8.25	8.36	
5	11.17	11.66	11.88	12.00	$\delta = 4$
6	14.70	15.07	15.28	15.36	
7	17.80	18.20	18.42	18.56	
8	23.22	24.09	24.61	24.93	
9	39.44	41.97	43.69	44.89	
1	3.25	3.26	3.27	3.28	
2	5.18	5.23	5.24	5.25	
3	7.73	7.92	7.98	8.01	
4	10.85	11.18	11.30	11.36	
5	14.31	14.70	14.85	14.92	$\delta = 8$
6	17.56	17.91	18.05	18.13	
7	20.86	21.38	21.62	21.75	
8	27.43	28.51	29.10	29.45	
9	46.27	49.36	51.37	52.75	

Radial concentration profiles under slip and no-slip condition at the wall are shown in Figs. 1 and 2 for $\beta = 0, 4, 12$ and $\delta = 4, 8$. Examination of these figures leads us to infer (i) that, whatever be the values of β and δ , presence of velocity slip at the boundary causes the concentration to increase in the entire cross-section of the tube; (ii) under both slip and no-slip conditions, the concentration decreases with increase in the reaction rate parameters; this is in agreement with results of references 8–10 which deal with the problem when no-slip condition holds at the boundary; (iii) variation in concentration is more sensitive to variation in the homogeneous reaction rate parameter δ vis-a-vis variation in β , under slip as well as no-slip condition at the boundary; (iv) when velocity slip at the porous wall is taken into account, the concentration profiles for different values of β and δ continue to retain the qualitative features similar to those of the profiles obtained under no-slip condition.

In situations where permeability of the porous surface is large, greater slip velocities would be obtained and this, in turn, would have a pronounced effect on concentration profiles. Thus the present study reveals that erroneous concentration profiles would result if slip effect were not incorporated in analysing the problem of dispersion in flows past porous surfaces.

Table 2. First nine eigenvalues λ_n under no-slip condition when $P_e = 100$.

n	β	λ				
		0	4	8	12	
1	0.98	1.04	1.06	1.06		
2	2.22	2.50	2.58	2.62		
3	4.47	4.94	5.09	5.17		
4	7.68	8.20	8.41	8.52		
5	11.38	11.99	12.10	12.21	$\delta = 4$	
6	14.95	15.34	15.52	15.62		
7	18.12	18.54	18.77	18.91		
8	23.80	24.73	25.27	25.61		
9	41.09	43.89	45.77	47.09		
1	3.28	3.29	3.30	3.31		
2	5.26	5.31	5.32	5.33		
3	7.88	8.06	8.12	8.15		
4	11.07	11.39	11.51	11.57		
5	14.58	14.97	15.11	15.19	$\delta = 8$	
6	17.88	18.22	18.36	18.43		
7	21.30	21.82	22.06	22.19		
8	28.19	29.33	29.94	30.31		
9	48.35	51.76	53.96	55.46		

Table 3. First nine eigenvalues λ_n in absence of chemical reactions ($\beta = 0$, $\delta = 0$) under no-slip and slip ($u_s/u_c = 0.0029$, $\alpha = 4$, $\sigma = 50$) conditions when $P_e = 100$

n	λ_n	
	no-slip	slip
1	0.00	0.00
2	1.04	1.02
3	3.33	3.27
4	6.59	6.46
5	10.35	10.16
6	14.00	13.76
7	17.13	16.84
8	22.44	21.92
9	38.78	37.29

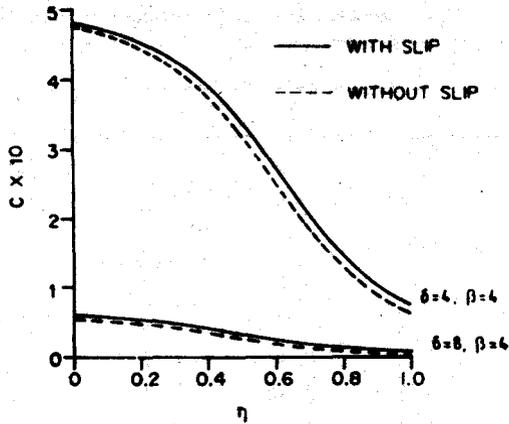


Figure 1. Variation in concentration with dimensionless radial distance co-ordinate at axial location $\xi = 1$ for $\beta = 4$, $\delta = 4, 8$. (with slip $\frac{u}{v} = 0.0029$ and without slip $\frac{u}{v} = 0$)

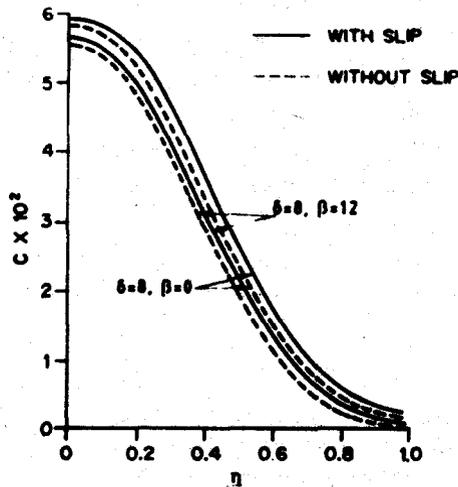


Figure 2. Variation in concentration with dimensionless radial distance co-ordinate at axial location $\xi = 1$ for $\beta = 0, 12$, $\delta = 8$. (with slip $\frac{u}{v} = 0.0029$ and without slip $\frac{u}{v} = 0$)

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