

Effects of Homogeneous and Heterogeneous Reactions on the Dispersion of a Solute for Immiscible Viscous Fluids between Two Plates

J. P. Kumar, J.C. Umavathi[†] and A. Basavaraj

Department of Mathematics, Gulbarga University, Gulbarga-585 106, India

[†]Corresponding Author Email: jc_uma11@yahoo.com

(Received February 18, 2010; accepted August 27, 2011)

ABSTRACT

The paper presents an analytical solution for the dispersion of a solute of two immiscible viscous fluids in the presence of an irreversible first-order chemical reaction. The effects of both homogeneous and heterogeneous reactions on the dispersion are studied. The results are presented graphically and in tabular form for various values of viscosity ratio and pressure gradients on the volumetric flow rate and effective Taylor dispersion coefficient. It is found that for homogeneous chemical reaction, the effective Taylor dispersion coefficient decreases as reaction rate parameter increases. The validity of the results obtained from an analytical method for two fluid models is verified by comparison with the available one fluid model results, and good agreement is found.

Keywords: Taylor dispersion, Homogeneous, Heterogeneous, Chemical reaction, Immiscible fluids, Diffusivity.

NOMENCLATURE

| | | | |
|---------------------|---|---|--|
| C_i | concentration of the solute (Kg m^{-3}) | p_i | dimensionless pressure gradients |
| D_i | molecular diffusion co-efficient ($\text{m}^2 \text{s}^{-1}$) | Y_i | space co-ordinates, (m) |
| K_i | first-order reaction rate constant (K^{-1}) | y_i | dimensionless space co-ordinates |
| L | typical length (m) | Greek symbols | |
| Q_i | volumetric flow rate ($\text{m}^3 \text{s}^{-1}$) | α_i, β_i | dimensionless reaction rate parameters |
| U_i | velocity (ms^{-1}) | η | dimensionless length |
| u_i | dimensionless velocity | μ_i | dynamic viscosity ($\text{Kg m}^{-1} \text{s}^{-1}$) |
| \bar{u}_i | average velocity (ms^{-1}) | ρ_i | density of the fluid (Kg m^{-3}) |
| $\frac{dP_i}{dX_i}$ | pressure gradient (Nm^{-2}) | Subscripts | |
| | | $i = 1, 2$ Where 1, 2 – quantities for region-1 and region-2, respectively. | |

1. INTRODUCTION

A wide application of the dispersion model began forty years ago when numerous authors noticed that longitudinal mixing can be treated the same as diffusion (see [Levenspiel et al. 1957](#)). The most notable is the work of [Danckwerts \(1953\)](#) and [Taylor \(1953, 1954a, 1954b\)](#) who in pioneering papers introduced the concept of longitudinal dispersion superimposed on plug flow to describe the fact that not all fluid elements travel at equal speed through a system.

[Taylor \(1953, 1954a\)](#) investigated the way in which a liquid spreads out longitudinally as it moves down a straight tube and demonstrated by a few careful experiments and a novel mathematical analysis of a

rather heuristic kind, that far downstream of the source the longitudinal spread is equivalent to a diffusion process; he also provided estimates for the longitudinal dispersion coefficient. Since then the notion of a longitudinal dispersion has been recognized as being relevant in a wide variety of contexts, like in flows in rivers and estuaries, in oil pipelines, in water mains, in pneumatic and hydraulic industrial devices, in blood vessels, in tubules in plants. An enormous variety of extensions and generalizations of Taylor's simple result for steady flow in a straight circular tube has been developed ([Batchelor, \(1981\)](#)). The most notable developments of the classical asymptotic theory of Taylor, while still preserving the basic ideas of his original work were produced by [Aris \(1956\)](#), [Horn \(1971\)](#), and [Brenner \(1980, 1982\)](#). Considerable

attention has also been paid to the one-dimensional dispersion of solute during relatively short times, too short for the macrotransport process to be fully established (Philip 1963; Gill *et al.* 1972; Hatton and Lightfoot 1982; Yamanaka 1983; Yamanaka *et al.* 1994). The importance for practice of the diffusion analysis of Taylor and the subsequent investigations lies in the ability of the one-dimensional transport equation to take into account complicated velocity and concentration profiles in a simpler manner, as well as providing a theoretical framework for the dispersion coefficient.

Taylor (1953) assumed that the solute does not chemically react with the fluid. However, in a variety of problems in chemical engineering, diffusion of solute takes place in the presence of irreversible first order chemical reaction. Therefore, many investigators analyzed the dispersion problem by considering first order homogeneous reaction, under laminar flow conditions. Further, the wall of the channel may be catalytic, which in turn gives rise to heterogeneous chemical reaction at the surface. Katz (1959) discussed the influence of the heterogeneous chemical reaction catalyzed on the wall of the tube. The combined effects of homogeneous and heterogeneous chemical reaction for a solute dispersing in Newtonian fluid flow have been discussed by Walker (1961), Solomon *et al.* (1967), Gupta *et al.* (1972) and others. Dutta *et al.* (1974) also discussed the non-Newtonian fluid with simultaneous chemical reaction. The influence of an applied magnetic field on the dispersion has been discussed recently by Narasimha Murthy *et al.* (1974). They found that the solute in an electrically conducting solvent can regulate rate of diffusion.

Problems involving multi-phase flow and heat transfer arise in a number of scientific and engineering disciplines. Important applications include petroleum industry, geophysics and plasma physics, in modeling such problems, the presence of second immiscible fluid phase adds a number of complexities as to the nature of interacting transport phenomena and interface conditions between the phases. In general multi-fluid flows are driven by gravitational and viscous flows. There has been some theoretical and experimental work on laminar flow of two immiscible fluids in a horizontal pipe (Aliareza *et al.* 1970). Umavathi *et al.* (2007, 2010), Malashetty *et al.* (2005, 2006) and Prathap *et al.* (2009, 2010) worked on two or three immiscible fluids.

Hence keeping in view the practical applications of immiscible fluids, it is the objective of this paper to analyze the dispersion of solute with simultaneous chemical reaction for two immiscible viscous fluids flowing in a channel using the approach due to Taylor (1953).

2. MATHEMATICAL FORMULATION

The physical configuration considered in this study is shown in Fig. 1. Consider the laminar flow of two immiscible fluids between two parallel plates distant $2h$ apart, taking X -axis along the mid-section of the channel and Y -axis perpendicular to the walls. Region-1 ($-h \leq Y \leq 0$) is filled with fluid saturated porous

medium of density ρ_1 , viscosity μ_1 , under a uniform pressure gradient $\frac{dP_1}{dX}$ whereas region-2 ($0 \leq Y \leq h$) is filled with another viscous fluid of density ρ_2 , viscosity μ_2 under a uniform pressure gradient $\frac{dP_2}{dX}$. The fluids in both the regions are Newtonian fluids.

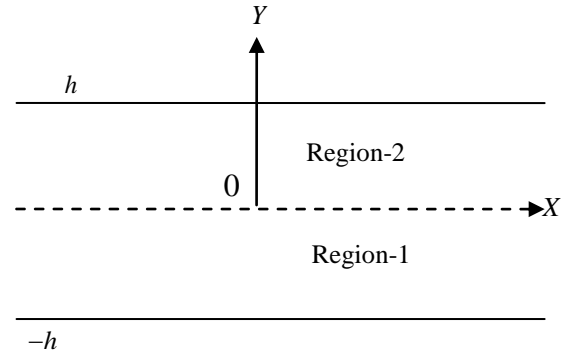


Fig. 1. Physical configuration.

It is assumed that the flow is steady, laminar, fully developed, and that fluid properties are constant. The flow in both regions is assumed to be driven by a common constant pressure gradient. Under these assumptions, the governing equations of motion for incompressible fluids are

Region-1

$$\frac{d^2 U_1}{dY^2} = \frac{1}{\mu_1} \frac{dP_1}{dX} \quad (1)$$

Region-2

$$\frac{d^2 U_2}{dY^2} = \frac{1}{\mu_2} \frac{dP_2}{dX} \quad (2)$$

where U_i is the X -component of fluid velocity and P_i is the pressure. The subscripts 1 and 2 denote the values for region-1 and region-2 respectively.

The boundary conditions on velocity are no-slip conditions requiring that the velocity must vanish at the walls. In addition, continuity of velocity and shear stress at the interface is assumed. With these assumptions, the boundary and interface conditions on velocity become

$$\begin{aligned} U_1 &= 0 \quad \text{at } Y = -h \\ U_2 &= 0 \quad \text{at } Y = h \\ U_1 &= U_2 \quad \text{at } Y = 0 \\ \mu_1 \frac{dU_1}{dY} &= \mu_2 \frac{dU_2}{dY} \quad \text{at } Y = 0 \end{aligned} \quad (3)$$

Using the non-dimensional parameters

$$\begin{aligned} \eta &= \frac{Y}{h}, \quad u_1 = \frac{\rho_1 h}{\mu_1} U_1, \quad u_2 = \frac{\rho_2 h}{\mu_2} U_2, \quad x = \frac{X}{h}, \\ p_1^* &= \frac{P_1}{\rho_1 (v_1 / h)^2}, \quad p_2^* = \frac{P_2}{\rho_2 (v_2 / h)^2} \end{aligned} \quad (4)$$

The Eqs. (1) to (3) become

$$\frac{d^2 u_1}{dy^2} = p_1 \quad (5)$$

$$\frac{d^2 u_2}{dy^2} = p_2 \quad (6)$$

$$\begin{aligned} u_1 &= 0 \quad \text{at } \eta = -1 \\ u_2 &= 0 \quad \text{at } \eta = 1 \\ u_1 &= mn u_2 \quad \text{at } \eta = 0 \end{aligned} \quad (7)$$

$$\frac{du_1}{d\eta} = m^2 n \frac{du_2}{d\eta} \quad \text{at } \eta = 0$$

where $p_1 = \frac{dp_1^*}{dx}$, $p_2 = \frac{dp_2^*}{dx}$, $m = \mu_2/\mu_1$ and $n = \rho_1/\rho_2$

Solutions of Eqs. (5) and (6) are

$$u_1 = \frac{p_1 \eta^2}{2} + a_1 \eta + a_2 \quad (8)$$

$$u_2 = \frac{p_2 \eta^2}{2} + a_3 \eta + a_4 \quad (9)$$

where a_1 , a_2 , a_3 and a_4 are integrating constants that are evaluated using boundary and interface conditions as given in (7).

From Eqs. (8) and (9) the average velocities become

$$\bar{u}_1 = \frac{1}{2} \int_{-1}^0 u_1 d\eta = \frac{1}{2} \left(\frac{p_1}{6} - \frac{a_1}{2} + a_2 \right) \quad (10)$$

$$\bar{u}_2 = \frac{1}{2} \int_0^1 u_2 d\eta = \frac{1}{2} \left(\frac{p_2}{6} + \frac{a_3}{2} + a_4 \right) \quad (11)$$

Case-1a: Diffusion with a homogeneous chemical reaction

We assume that a solute diffuses and simultaneously undergoes a first-order irreversible chemical reaction in the liquid under isothermal conditions. The equation for the concentration C_1 of the solute for the region-1 satisfies

$$\frac{\partial C_1}{\partial t} + u_1 \frac{\partial C_1}{\partial X} = D_1 \left(\frac{\partial^2 C_1}{\partial X^2} + \frac{\partial^2 C_1}{\partial Y^2} \right) - K_1 C_1 \quad (12)$$

Similarly, the equation for the concentration C_2 of the solute for the region-2 satisfies

$$\frac{\partial C_2}{\partial t} + u_2 \frac{\partial C_2}{\partial X} = D_2 \left(\frac{\partial^2 C_2}{\partial X^2} + \frac{\partial^2 C_2}{\partial Y^2} \right) - K_2 C_2 \quad (13)$$

in which D_1 and D_2 are the molecular diffusion coefficients (assumed constant) for the region-1 and region-2 respectively and K_1 and K_2 are the first-order reaction rate constants. In deriving the Eqs. (12) and (13), it is assumed that the solute is present in a small concentration, the last term $-K_1 C_1 / \text{mol m}^{-3} \text{s}^{-1}$ and $-K_2 C_2 / \text{mol m}^{-3} \text{s}^{-1}$ represents the volume rate of disappearance of the solute due to chemical reaction. We now assume that

$$\frac{\partial^2 C_1}{\partial X^2} \ll \frac{\partial^2 C_1}{\partial Y^2} \quad \text{and} \quad \frac{\partial^2 C_2}{\partial X^2} \ll \frac{\partial^2 C_2}{\partial Y^2}.$$

If we now consider convection across a plane moving with the mean speed of the flow, then relative to this plane the fluid velocities are given by

Region-1

$$u_{1x} = u_1 - \bar{u} = \frac{p_1 \eta^2}{2} + a_1 \eta + lc_1 \quad (14)$$

Region-2

$$u_{2x} = u_2 - \bar{u} = \frac{p_2 \eta^2}{2} + a_3 \eta + lc_2 \quad (15)$$

where \bar{u} is the sum of average velocities of region-1 and region-2.

Introducing the dimensionless quantities

$$\begin{aligned} \theta_1 &= \frac{t}{t_1}, \quad \bar{t}_1 = \frac{L}{u_1}, \quad \theta_2 = \frac{t}{t_2}, \quad \bar{t}_2 = \frac{L}{u_2}, \\ \xi_1 &= \frac{x_1 - \bar{u}_1 t}{L_1}, \quad \xi_2 = \frac{x_2 - \bar{u}_2 t}{L}, \quad \eta = \frac{Y}{h} \end{aligned} \quad (16)$$

and using Eq (16), Eqs. (12) and (13) becomes

Region-1

$$\frac{1}{t} \frac{\partial C_1}{\partial \theta_1} + \frac{u_{1x}}{L} \frac{\partial C_1}{\partial \xi} = \frac{D_1}{h^2} \frac{\partial^2 C_1}{\partial \eta^2} - K_1 C_1 \quad (17)$$

Region-2

$$\frac{1}{t} \frac{\partial C_2}{\partial \theta_2} + \frac{u_{2x}}{L} \frac{\partial C_2}{\partial \xi} = \frac{D_2}{h^2} \frac{\partial^2 C_2}{\partial \eta^2} - K_2 C_2 \quad (18)$$

where L is the typical length along the flow direction. Following Taylor (1953), we now assume that partial equilibrium is established in any cross-section of the channel so that the variations of C_1 and C_2 with η are calculated from Eqs. (17) and (18) as

Region-1

$$\frac{\partial^2 C_1}{\partial \eta^2} - \alpha_1^2 C_1 = \frac{h^2}{D_1 L} u_{1x} \frac{\partial C_1}{\partial \xi} \quad (19)$$

Region-2

$$\frac{\partial^2 C_2}{\partial \eta^2} - \alpha_2^2 C_2 = \frac{h^2}{D_2 L} u_{2x} \frac{\partial C_2}{\partial \xi} \quad (20)$$

where $\alpha_1 = h\sqrt{K_1/D_1}$ and $\alpha_2 = h\sqrt{K_2/D_2}$

To solve Eqs. (19) and (20) we use wall boundary conditions, namely

$$\frac{\partial C_1}{\partial \eta} = 0 \quad \text{at } \eta = -1 \quad \text{and} \quad \frac{\partial C_2}{\partial \eta} = 0 \quad \text{at } \eta = 1 \quad (21)$$

To find the solutions of Eqs. (19) and (20), we require two more interface conditions along with boundary condition (21) which are given by

$$C_1 = C_2 \quad \text{and} \quad D_1 \frac{\partial C_1}{\partial \eta} = D_2 \frac{\partial C_2}{\partial \eta} \quad \text{at } \eta = 0 \quad (22)$$

Equations (19) and (20) are solved for C_1 and C_2 which are given by

Region-1

$$C_1 = b_1 \cosh(\alpha_1 \eta) + b_2 \sinh(\alpha_1 \eta) + \frac{h^2}{D_1 L} \frac{\partial C_1}{\partial \xi_1} (l_1 \eta^2 + l_2 \eta + l_3) \quad (23)$$

Region-2

$$C_2 = b_3 \cosh(\alpha_2 \eta) + b_4 \sinh(\alpha_2 \eta) + \frac{h^2}{D_2 L} \frac{\partial C_2}{\partial \xi_2} (l_4 \eta^2 + l_5 \eta + l_6) \quad (24)$$

where b_1, b_2, b_3 and b_4 are the integrating constants which are evaluated using boundary and interface conditions as defined in Eqs. (21) and (22). The expressions for C_1 and C_2 can also written as

$$C_1 = \frac{h^2}{D_1 L} \frac{\partial C_1}{\partial \xi_1} C_{11} + \frac{h^2}{D_2 L} \frac{\partial C_2}{\partial \xi_2} C_{12}$$

$$C_2 = \frac{h^2}{D_1 L} \frac{\partial C_1}{\partial \xi_1} C_{21} + \frac{h^2}{D_2 L} \frac{\partial C_2}{\partial \xi_2} C_{22}$$

where

$$C_{11} = b_{11} \cosh(\alpha_1 \eta) + b_{21} \sinh(\alpha_1 \eta) + l_1 \eta^2 + l_2 \eta + l_3$$

$$C_{12} = b_{12} \cosh(\alpha_1 \eta) + b_{22} \sinh(\alpha_1 \eta)$$

$$C_{21} = b_{31} \cosh(\alpha_2 \eta) + b_{41} \sinh(\alpha_2 \eta)$$

$$C_{22} = b_{32} \cosh(\alpha_2 \eta) + b_{42} \sinh(\alpha_2 \eta) + l_4 \eta^2 + l_5 \eta + l_6$$

The volumetric flow rates at which the solute is transported across a section of the channel of unit breadth Q_1 (region-1) and Q_2 (region-2) using Eqs. (14), (15) and (23), (24) are

Region-1

$$Q_1 = h \int_{-1}^0 C_1 u_{1x} d\eta = -(Q_{11} + Q_{12}) \quad (25)$$

$$\text{where } Q_{11} = -\frac{h^3}{D_1 L} \frac{\partial C_1}{\partial \xi_1} \int_{-1}^0 C_{11} u_{1x} d\eta$$

$$\text{and } Q_{12} = -\frac{h^3}{D_2 L} \frac{\partial C_2}{\partial \xi_2} \int_{-1}^0 C_{12} u_{1x} d\eta$$

Region-2

$$Q_2 = h \int_0^1 C_2 u_{2x} d\eta = -(Q_{21} + Q_{22}) \quad (26)$$

$$\text{where } Q_{21} = -\frac{h^3}{D_1 L} \frac{\partial C_1}{\partial \xi_1} \int_0^1 C_{21} u_{2x} d\eta$$

$$\text{and } Q_{22} = -\frac{h^3}{D_2 L} \frac{\partial C_2}{\partial \xi_2} \int_0^1 C_{22} u_{2x} d\eta$$

Following Taylor (1953), we assume that the variations of C_1 and C_2 with η are small compared with those in the longitudinal direction, and if C_{m1} and C_{m2} are the mean concentration over a section, $\partial C_1 / \partial \xi_1$ and

$\partial C_2 / \partial \xi_2$ are indistinguishable from $\partial C_{m1} / \partial \xi_1$ and $\partial C_{m2} / \partial \xi_2$ respectively so that Eqs. (26) and (27) may be written as

Region-1

$$Q_{11} = -D_{11}^* \frac{\partial C_{m1}}{\partial \xi_1}, \quad Q_{12} = -D_{12}^* \frac{\partial C_{m2}}{\partial \xi_2}$$

Region-2

$$Q_{21} = -D_{21}^* \frac{\partial C_{m1}}{\partial \xi_1} \quad \text{and} \quad Q_{22} = -D_{22}^* \frac{\partial C_{m2}}{\partial \xi_2}$$

The fact that no material is lost in the process is expressed by the continuity equation for C_{m1} and C_{m2} , namely

Region-1

$$\frac{\partial Q_{11}}{\partial \xi_1} = -2 \frac{\partial C_{m1}}{\partial t}, \quad \frac{\partial Q_{12}}{\partial \xi_2} = -2 \frac{\partial C_{m2}}{\partial t} \quad (27)$$

Region-2

$$\frac{\partial Q_{21}}{\partial \xi_1} = -2 \frac{\partial C_{m1}}{\partial t}, \quad \frac{\partial Q_{22}}{\partial \xi_2} = -2 \frac{\partial C_{m2}}{\partial t} \quad (28)$$

Equations (27) and (28) using Eqs. (25) and (26) become

Region-1

$$\frac{\partial C_{m1}}{\partial t} = \frac{D_{11}^*}{4} \frac{\partial^2 C_{m1}}{\partial \xi_1^2}, \quad \frac{\partial C_{m2}}{\partial t} = \frac{D_{12}^*}{4} \frac{\partial^2 C_{m2}}{\partial \xi_2^2} \quad (29)$$

Region-2

$$\frac{\partial C_{m1}}{\partial t} = \frac{D_{21}^*}{4} \frac{\partial^2 C_{m1}}{\partial \xi_1^2}, \quad \frac{\partial C_{m2}}{\partial t} = \frac{D_{22}^*}{4} \frac{\partial^2 C_{m2}}{\partial \xi_2^2} \quad (30)$$

which are the equations governing the longitudinal dispersion, where

$$D_{11}^* = \frac{h^2}{2D_1} \int_{-1}^0 C_{11} u_{1x} d\eta = \frac{h^2}{2D_1} F_{11}(p_1, p_2, \alpha_1, \alpha_2, m, n)$$

$$D_{12}^* = \frac{h^2}{2D_2} \int_{-1}^0 C_{12} u_{1x} d\eta = \frac{h^2}{2D_2} F_{12}(p_1, p_2, \alpha_1, \alpha_2, m, n)$$

$$D_{21}^* = \frac{h^2}{2D_1} \int_0^1 C_{21} u_{2x} d\eta = \frac{h^2}{2D_1} F_{21}(p_1, p_2, \alpha_1, \alpha_2, m, n)$$

$$D_{22}^* = \frac{h^2}{2D_2} \int_0^1 C_{22} u_{2x} d\eta = \frac{h^2}{2D_2} F_{22}(p_1, p_2, \alpha_1, \alpha_2, m, n)$$

Values of F_{ii} are computed for different values of dimensionless parameters such as viscosity ratio m and pressure gradients p_1, p_2 for variations of α_1 and α_2 and are shown in Table 1. Volumetric flow rate is also computed for variations of viscosity ratio and pressure gradients are displayed in Fig. 2.

Table 1 Values of effective dispersion coefficient for variations of viscosity ratio and pressure gradients for homogeneous chemical reaction.

| | | $m = 0.1$ | | | $m = 1$ | | |
|----------|---------------------------|---------------------------|-------------------------|---------------------------|---------------------------|-------------------------|--|
| α | $F_1(\alpha_1, \alpha_2)$ | $F_2(\alpha_1, \alpha_2)$ | $F(\alpha_1, \alpha_2)$ | $F_1(\alpha_1, \alpha_2)$ | $F_2(\alpha_1, \alpha_2)$ | $F(\alpha_1, \alpha_2)$ | |
| 0.4 | 0.1351300 | 0.1191240 | 0.2542540 | 0.0010415 | 0.0010415 | 0.0020831 | |
| 0.8 | 0.1153070 | 0.1091580 | 0.2244650 | 9.94588E-4 | 9.94588E-4 | 0.0019892 | |
| 1.2 | 0.0929812 | 0.0969963 | 0.1899775 | 9.25165E-4 | 9.25165E-4 | 0.0018503 | |
| 1.6 | 0.0735110 | 0.0851309 | 0.1586419 | 8.42935E-4 | 8.42935E-4 | 0.0016859 | |
| 2 | 0.0582265 | 0.0745092 | 0.1327357 | 7.56654E-4 | 7.56654E-4 | 0.0015133 | |
| | | $m = 2$ | | | $p_1 = p_2 = -5$ | | |
| α | $F_1(\alpha_1, \alpha_2)$ | $F_2(\alpha_1, \alpha_2)$ | $F(\alpha_1, \alpha_2)$ | $F_1(\alpha_1, \alpha_2)$ | $F_2(\alpha_1, \alpha_2)$ | $F(\alpha_1, \alpha_2)$ | |
| 0.4 | 0.0024974 | 0.0027925 | 0.0052899 | 0.0260385 | 0.0260385 | 0.0520770 | |
| 0.8 | 0.0024023 | 0.0024623 | 0.0048647 | 0.0248647 | 0.0248647 | 0.0497294 | |
| 1.2 | 0.0022571 | 0.0020761 | 0.0043332 | 0.0231291 | 0.0231291 | 0.0462582 | |
| 1.6 | 0.0020799 | 0.0017207 | 0.0038005 | 0.0210734 | 0.0210734 | 0.0421467 | |
| 2 | 0.0018891 | 0.0014234 | 0.0033125 | 0.0189163 | 0.0189163 | 0.0378327 | |
| | | $p_1 = p_2 = 0.1$ | | | $p_1 = p_2 = 5$ | | |
| α | $F_1(\alpha_1, \alpha_2)$ | $F_2(\alpha_1, \alpha_2)$ | $F(\alpha_1, \alpha_2)$ | $F_1(\alpha_1, \alpha_2)$ | $F_2(\alpha_1, \alpha_2)$ | $F(\alpha_1, \alpha_2)$ | |
| 0.4 | 1.04154E-5 | 1.04154E-5 | 2.08308E-5 | 0.0260385 | 0.0260385 | 0.0520770 | |
| 0.8 | 9.94587E-6 | 9.94587E-6 | 1.98918E-5 | 0.0248647 | 0.0248647 | 0.0497294 | |
| 1.2 | 9.25164E-6 | 9.25164E-6 | 1.85033E-5 | 0.0231291 | 0.0231291 | 0.0462582 | |
| 1.6 | 8.42934E-6 | 8.42934E-6 | 1.68587E-5 | 0.0210734 | 0.0210734 | 0.0421467 | |
| 2 | 7.56653E-6 | 7.56653E-6 | 1.51331E-5 | 0.0189163 | 0.0189163 | 0.0378327 | |

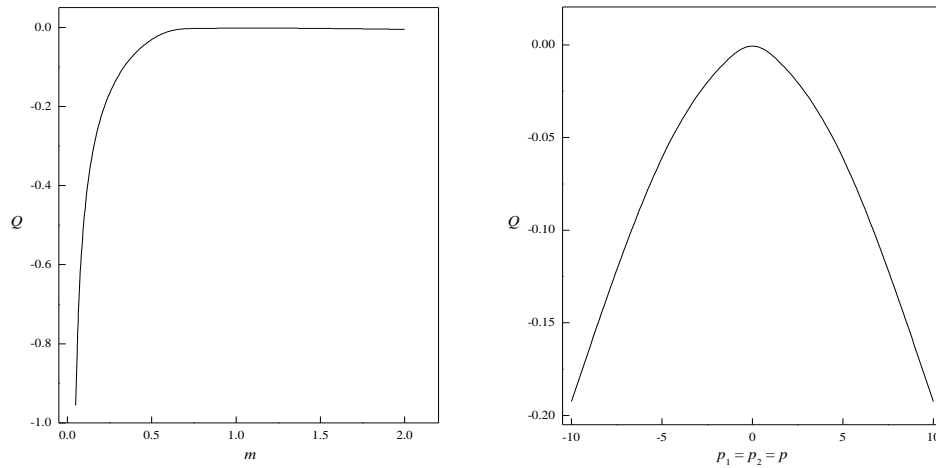


Fig. 2. Volumetric flow rate Q profiles for homogeneous impermeable wall conditions

Case 1b: Diffusion with combined homogeneous and heterogeneous chemical reaction

We now discuss the problem of diffusion in a channel with a first-order irreversible chemical reaction taking place both in the bulk of the fluid as well as at the walls which are assumed to be catalytic. In this case the diffusion equations remain the same as defined in Eqs. (19) and (20) subject to the dimensionless boundary and interface conditions as

$$\begin{aligned}
 \frac{\partial C_1}{\partial \eta} - \beta_1 C_1 &= 0 \quad \text{at } \eta = -1 \\
 \frac{\partial C_2}{\partial \eta} + \beta_2 C_2 &= 0 \quad \text{at } \eta = 1 \\
 C_1 = C_2 &\quad \text{at } \eta = 0 \\
 D_1 \frac{\partial C_1}{\partial \eta} = D_2 \frac{\partial C_2}{\partial \eta} &\quad \text{at } \eta = 0
 \end{aligned}
 \tag{31}$$

Where $\beta_1 = f_1 h$ and $\beta_2 = f_2 h$ are the heterogeneous reaction rate parameters corresponding to catalytic reaction at the walls.

The solutions of Eqs. (19) and (20) are

Region-1

$$C_1 = b_1 \cosh(\alpha_1 \eta) + b_2 \sinh(\alpha_1 \eta) + \frac{h^2}{D_1 L} \frac{\partial C_1}{\partial \xi_1} (l_1 \eta^2 + l_2 \eta + l_3) \quad (32)$$

Region-2

$$C_2 = b_3 \cosh(\alpha_2 \eta) + b_4 \sinh(\alpha_2 \eta) + \frac{h^2}{D_2 L} \frac{\partial C_2}{\partial \xi_2} (l_4 \eta^2 + l_5 \eta + l_6) \quad (33)$$

Where b_1, b_2, b_3 and b_4 are the integrating constants obtained using boundary and interface conditions as defined in Eq. (31).

The volumetric rates at which the solute is transported across a section of the channel of unit breadth Q_1 (region-1) and Q_2 (region-2) and the evaluation of effective dispersion coefficients F_{ii} are evaluated as explained in the case 1a and tabulated in Table 2.

Table 2 Values of effective dispersion coefficient for variations of viscosity ratio and pressure gradients for combined homogeneous and heterogeneous chemical reaction

| | | $m = 0.1$ | | | $m = 1$ | | |
|---------|--|--------------------------|--------------------------|------------------------|--------------------------|--------------------------|------------------------|
| β | | $F_1(\alpha_i, \beta_i)$ | $F_2(\alpha_i, \beta_i)$ | $F(\alpha_i, \beta_i)$ | $F_1(\alpha_i, \beta_i)$ | $F_2(\alpha_i, \beta_i)$ | $F(\alpha_i, \beta_i)$ |
| 2 | | 0.0393615 | 0.1189920 | 0.1583535 | 8.48463E-4 | 8.48463E-4 | 0.0016969 |
| 4 | | 0.0258395 | 0.1209060 | 0.1467455 | 8.30289E-4 | 8.30289E-4 | 0.0016606 |
| 6 | | 0.0199143 | 0.1216090 | 0.1415233 | 8.22866E-4 | 8.22866E-4 | 0.0016457 |
| 8 | | 0.0165837 | 0.1219700 | 0.1385537 | 8.18832E-4 | 8.18832E-4 | 0.0016377 |
| 10 | | 0.0144489 | 0.1221880 | 0.1366369 | 8.16298E-4 | 8.16298E-4 | 0.0016326 |
| | | $m = 2$ | | | $p_1 = p_2 = -5$ | | |
| β | | $F_1(\alpha_i, \beta_i)$ | $F_2(\alpha_i, \beta_i)$ | $F(\alpha_i, \beta_i)$ | $F_1(\alpha_i, \beta_i)$ | $F_2(\alpha_i, \beta_i)$ | $F(\alpha_i, \beta_i)$ |
| 2 | | 0.0029753 | 8.39576E-4 | 0.0038149 | 0.0212116 | 0.0212116 | 0.0424231 |
| 4 | | 0.0030907 | 5.59314E-4 | 0.0036500 | 0.0207572 | 0.0207572 | 0.0415144 |
| 6 | | 0.0031394 | 4.38321E-4 | 0.0035778 | 0.0205717 | 0.0205717 | 0.0411433 |
| 8 | | 0.0031664 | 3.70775E-4 | 0.0035372 | 0.0204708 | 0.0204708 | 0.0409416 |
| 10 | | 0.0031835 | 3.27649E-4 | 0.0035111 | 0.0204074 | 0.0204074 | 0.0408149 |
| | | $p_1 = p_2 = 0.1$ | | | $p_1 = p_2 = 5$ | | |
| β | | $F_1(\alpha_i, \beta_i)$ | $F_2(\alpha_i, \beta_i)$ | $F(\alpha_i, \beta_i)$ | $F_1(\alpha_i, \beta_i)$ | $F_2(\alpha_i, \beta_i)$ | $F(\alpha_i, \beta_i)$ |
| 2 | | 8.48463E-6 | 8.48463E-6 | 1.69693E-5 | 0.0212116 | 0.0212116 | 0.0424231 |
| 4 | | 8.30289E-6 | 8.30289E-6 | 1.66058E-5 | 0.0207572 | 0.0207572 | 0.0415144 |
| 6 | | 8.22866E-6 | 8.22866E-6 | 1.64573E-5 | 0.0205717 | 0.0205717 | 0.0411433 |
| 8 | | 8.18832E-6 | 8.18832E-6 | 1.63766E-5 | 0.0204708 | 0.0204708 | 0.0409416 |
| 10 | | 8.16298E-6 | 8.16298E-6 | 1.6326E-5 | 0.0204074 | 0.0204074 | 0.0408149 |

Case 2: Diffusion with combined homogeneous and heterogeneous chemical reaction (one fluid model)

The following are the solutions of one fluid model obtained by Gupta and Gupta (1972).

The non-dimensional equation of motion is

$$\frac{d^2 u}{d\eta^2} = \frac{dp}{dx} \quad (34)$$

along with boundary conditions

$$u = 0 \quad \text{at} \quad \eta = \pm 1 \quad (35)$$

The solution of Eq. (34) is

$$u = -p(1 - \eta^2)/2$$

The average velocity is given by

$$\bar{u} = -p/3$$

The concentration equation for one fluid model using Taylor (1953) become

$$\frac{\partial^2 C}{\partial \eta^2} - \alpha^2 C = \frac{h^2}{DL} \frac{\partial C}{\partial \xi} u_x \quad (36)$$

Where $u_x = \frac{p\eta^2}{2} - \frac{p}{6}$

The solution of Eq. (36) using boundary conditions

$$\frac{\partial C}{\partial \eta} = 0 \quad \text{at} \quad \eta = \pm 1 \quad \text{is}$$

$$C = A \cosh(\alpha \eta) - \frac{h^2}{\alpha^2 DL} \frac{\partial C}{\partial \xi} \left(\frac{p}{2} \eta^2 - \frac{p}{6} + \frac{p}{\alpha^2} \right) \quad (37)$$

The volumetric flow rate in which the solute is transported across a section of the channel of unit breadth is

$$Q = h \int_{-1}^1 C u_x d\eta = \frac{h^2 p^2}{\alpha^2 D} \frac{\partial C}{\partial \xi} \left(\frac{1}{\alpha^4} + \frac{1}{3\alpha^2} - \frac{1}{45} - \frac{\coth(\alpha)}{\alpha} \right) \quad (38)$$

Comparing Eq. (38) with Fick's law of diffusion, we find that the solute is dispersed relative to a plane moving with the mean speed of the flow with an effective dispersion coefficient D^* given by

$$D^* = \frac{h^2 p^2}{D} F(\alpha)$$

Where:

$$F(\alpha) = \frac{1}{\alpha^2} \left(\frac{\coth(\alpha)}{\alpha} - \frac{1}{\alpha^4} - \frac{1}{3\alpha^2} + \frac{1}{45} \right) \quad (39)$$

Values of $F(\alpha)$ are computed for different values of the dimensionless reaction rate parameter α and are shown in Table 3. When $\alpha \rightarrow 0$, Eq. (39) gives

$$\lim_{\alpha \rightarrow 0} F(\alpha) = \frac{2}{945}$$

So that the value for D^* can be written as $\frac{h^2 p^2}{D} \frac{2}{945}$

which agrees with the results of Wooding (1960) where p is non-dimensional pressure gradient. The solution for heterogeneous chemical reaction is also found for one fluid model and the results are shown in Table 4.

Table 3 Values of volumetric flow rate (Q) and effective dispersion coefficient for homogeneous chemical reaction.

| | Two fluid model | | | One fluid model |
|----------|---------------------------|---------------------------|-------------------------|-----------------|
| | Q_1 | Q_2 | Q | Q |
| | -9.62087E-4 | -9.62087E-4 | -0.0019242 | -0.0019242 |
| α | $F_1(\alpha_1, \alpha_2)$ | $F_2(\alpha_1, \alpha_2)$ | $F(\alpha_1, \alpha_2)$ | $F(\alpha)$ |
| 0.4 | 0.00104154 | 0.00104154 | 0.00208308 | 0.00208308 |
| 0.8 | 9.94588E-4 | 9.94588E-4 | 0.00198918 | 0.00198918 |
| 1.2 | 9.25165E-4 | 9.25165E-4 | 0.00185033 | 0.00185033 |
| 1.6 | 8.42935E-4 | 8.42935E-4 | 0.00168587 | 0.00168587 |
| 2 | 7.56654E-4 | 7.56654E-4 | 0.00151331 | 0.00151331 |

Table 4 Values of volumetric flow rate (Q) and effective dispersion coefficient for combined homogeneous and heterogeneous chemical reaction.

| | Two fluid model | | | One fluid model |
|---------|--------------------------|--------------------------|------------------------|--------------------|
| | Q_1 | Q_2 | Q | Q |
| | -8.73024E-4 | -8.73024E-4 | -0.0017461 | -0.0017461 |
| β | $F_1(\alpha_i, \beta_i)$ | $F_2(\alpha_i, \beta_i)$ | $F(\alpha_i, \beta_i)$ | $F(\alpha, \beta)$ |
| 2 | 8.48463E-4 | 8.48463E-4 | 0.0016969 | 0.0016969 |
| 4 | 8.30289E-4 | 8.30289E-4 | 0.0016606 | 0.0016606 |
| 6 | 8.22866E-4 | 8.22866E-4 | 0.0016457 | 0.0016457 |
| 8 | 8.18832E-4 | 8.18832E-4 | 0.0016377 | 0.0016377 |
| 10 | 8.16298E-4 | 8.16298E-4 | 0.0016326 | 0.0016326 |

All the constants appeared above are defined in the appendix.

3. RESULTS AND DISCUSSION

The problem concerned is with the longitudinal dispersion of a solute subject to molecular diffusion when it is introduced into a channel for viscous medium following Taylor's dispersion model with a homogeneous and heterogeneous first-order chemical reaction.

In order to find out average velocity in both the regions, no-slip conditions at the boundaries and continuity of velocity and shear stress is assumed at the interface. The volumetric flow rates in both the regions of the channel are also found. The effective dispersion coefficient in the each region is also evaluated and the values are tabulated for variations of governing parameters for homogeneous first-order chemical reaction. The effective dispersion coefficient is also found with a heterogeneous first-order chemical reaction. The physical parameters such as viscosity ratio and pressure gradients are fixed as one except the varying parameters in all the tabulated values.

Case-1a: Diffusion with a homogeneous chemical reaction

The effects of viscosity ratio and pressure gradients on volumetric flow rate are shown in Fig. 2. It is seen that as the viscosity ratio increases volumetric flow rate increases for small values of m and remains almost constant for values of viscosity ratio m greater than 0.75. Volumetric flow rate is symmetric for negative and positive values of pressure gradient $p (= p_1 = p_2)$ and the optimum flow rate is attained in the absence of pressure gradients.

The effective dispersion coefficients $F_1(\alpha_1, \alpha_2)$ (region-1) and $F_2(\alpha_1, \alpha_2)$ (region-2) for variations of viscosity ratio m and pressure gradient p is shown in Table 1. As the reaction rate parameter $\alpha (= \alpha_1 = \alpha_2)$ increases, $F_1(\alpha_1, \alpha_2)$ and $F_2(\alpha_1, \alpha_2)$ decreases in both the regions for any value of viscosity ratio m and pressure gradient p . The decrease in $F (= F_1 + F_2)$

with an increase in α is natural on physical grounds since an increase in α leads to an increase in the number of molecules of solute undergoing chemical reaction, resulting in a decrease in Taylor's dispersion coefficient. As m increases, the total effective dispersion coefficient decreases for $m \leq 1$ and increases for $m \geq 1$. The total effective dispersion coefficient $F(=F_1 + F_2)$ decreases as p increases for values of $p < 0$ and increases as p increases for values of $p > 0$. In the absence of pressure gradient p the values of F are very small and is of order 10^{-5} .

Case 1b: Diffusion with combined homogeneous and heterogeneous chemical reaction

The effect of viscosity ratio and pressure gradients on volumetric flow rate is similar to the effect of homogeneous chemical reaction and hence not displayed graphically.

The effects of heterogeneous reaction rate parameter β for a fixed value of homogeneous reaction rate parameter α are tabulated in Table 2. From this it is clear that as in the case of homogeneous reaction, the increase in the wall catalytic parameter causes decrease in the effective dispersion coefficient for all values of viscosity ratio m and pressure gradient p . Further as the viscosity ratio increases the total effective dispersion coefficient F decreases, whereas as the pressure gradients p increases F decreases for $p \leq 0$ and increases for $p \geq 0$.

Case 2: Diffusion with combined homogeneous and heterogeneous chemical reaction (one fluid model)

The problem of Gupta *et al.* (1972) is solved and compared the results. It is seen from Tables 3 and 4 that the values of volumetric flow rate and effective dispersion coefficient agree very well (two fluid model) with the results of Gupta *et al.* (1972) for one fluid model which justify the two fluid model for both homogeneous and heterogeneous chemical reactions.

The volumetric flow rate and effective dispersion coefficient are evaluated for variations homogeneous and heterogeneous reaction rate parameters for two and one fluid model and shown in Tables 3 and 4. The values of volumetric flow rate and effective dispersion coefficient tally with the results of Gupta *et al.* (1972).

4. CONCLUSION

The problem of solute dispersion of a solute in a viscous fluid between two parallel plates was studied using Taylor's dispersion model in the presence of first order homogeneous and heterogeneous chemical reaction for two fluid models.

The results obtained for homogeneous first-order chemical reactions were:

As the homogeneous reaction rate parameter increases, the effective dispersion coefficient decreases. The effective dispersion coefficient decreases for values of viscosity ratio and pressure gradients less than one and

increases for values of viscosity ratio and pressure gradients greater than one.

The results obtained for heterogeneous first-order chemical reactions were:

As the wall catalytic parameter increases, the effective dispersion coefficient decreases. The effect of viscosity ratio was to reduce the effective dispersion coefficient. The effect of pressure gradient on the effective dispersion coefficient was similar to the results observed for homogeneous chemical reactions.

The volumetric flow rate increases in magnitude as the viscosity ratio increases for small values and then remained invariant for large values for both homogeneous and heterogeneous wall boundary conditions whereas it is symmetric on pressure gradients.

ACKNOWLEDGEMENTS

The authors thank UGC-New Delhi for the financial support under UGC-Major Research Project.

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APPENDIX

Case-1a: Diffusion with a Homogeneous Chemical Reaction

$$u_1 = \frac{p_1 \eta^2}{2} + a_1 \eta + a_2, \quad u_2 = \frac{p_2 \eta^2}{2} + a_3 \eta + a_4$$

$$a_1 = -a_4 + \frac{p_2}{2}, \quad a_2 = m n a_4, \quad a_3 = -a_4 - \frac{p_2}{2},$$

$$a_4 = \frac{-p_1}{2mn(m+1)} - \frac{-p_2 m}{2(m+1)}$$

$$\bar{u}_1 = \frac{1}{2} \left(\frac{p_1}{6} - \frac{a_1}{2} + a_2 \right), \quad \bar{u}_2 = \frac{1}{2} \left(\frac{p_2}{6} + \frac{a_3}{2} + a_4 \right)$$

$$lc_1 = -\frac{1}{2} \left(\frac{p_1}{6} - \frac{a_1}{2} - a_2 + \frac{p_2}{6} + \frac{a_3}{2} + a_4 \right)$$

$$lc_2 = -\frac{1}{2} \left(\frac{p_1}{6} - \frac{a_1}{2} + a_2 + \frac{p_2}{6} + \frac{a_3}{2} - a_4 \right)$$

$$u_{1x} = \frac{p_1 \eta^2}{2} + a_1 \eta + lc_1, \quad u_{2x} = \frac{p_2 \eta^2}{2} + a_3 \eta + lc_2$$

$$l_1 = \frac{-p_1}{2\alpha_1^2}, \quad l_2 = \frac{-a_1}{\alpha_1^2}, \quad l_3 = -\frac{lc_1}{\alpha_1^2} - \frac{p_1}{\alpha_1^4}, \quad l_4 = \frac{-p_2}{2\alpha_2^2},$$

$$l_5 = \frac{-a_3}{\alpha_2^2}, \quad l_6 = -\frac{lc_2}{\alpha_2^2} - \frac{p_2}{\alpha_2^4},$$

$$Z_1 = \frac{h^2}{D_1 L} \frac{\partial C_1}{\partial \xi_1}, \quad Z_2 = \frac{h^2}{D_2 L} \frac{\partial C_2}{\partial \xi_2}$$

$$b_1 = Z_1 b_{11} + Z_2 b_{12}, \quad b_2 = Z_1 b_{21} + Z_2 b_{22}, \quad b_3 = Z_1 b_{31} + Z_2 b_{32}, \\ b_4 = Z_1 b_{41} + Z_2 b_{42}$$

$$Dr = \alpha_1 \alpha_2 \sinh(\alpha_1) \cosh(\alpha_2) \\ + \alpha_2^2 D \sinh(\alpha_2) \cosh(\alpha_1)$$

$$b_{41} = \frac{-\alpha_2 \sinh(\alpha_2) \left(l_3 \alpha_1 \sinh(\alpha_1) - l_2 \cosh(\alpha_1) \right)}{\text{Dr} \left(+l_2 - 2l_1 \right)}$$

$$b_{42} = \frac{-\sinh(\alpha_2) \left(\alpha_1 (l_5 + 2l_4) - l_6 \alpha_1 \alpha_2 \sinh(\alpha_1) \right)}{\text{Dr} \left(+l_5 D \alpha_2 \cosh(\alpha_1) \right)}$$

$$b_{31} = \frac{-b_{41}}{\tanh(\alpha_2)}, \quad b_{32} = \frac{-b_{42} \alpha_2 \cosh(\alpha_2) - 2l_4 - l_5}{\alpha_2 \sinh(\alpha_2)}$$

$$b_{11} = b_{31} - l_3, \quad b_{12} = b_{32} + l_6$$

$$b_{21} = \frac{b_{11} \alpha_1 \sinh(\alpha_1) + 2l_1 - l_2}{\alpha_1 \cosh(\alpha_1)}, \quad b_{22} = b_{12} \tanh(\alpha_1)$$

Case-1b: Diffusion with Combined Homogeneous and Heterogeneous Chemical Reaction

$$Z_1 = \frac{h^2}{D_1 L} \frac{\partial C_1}{\partial \xi_1}, \quad Z_2 = \frac{h^2}{D_2 L} \frac{\partial C_2}{\partial \xi_2}$$

$$b_1 = Z_1 b_{11} + Z_2 b_{12}, \quad b_2 = Z_1 b_{21} + Z_2 b_{22}, \quad b_3 = Z_1 b_{31} + Z_2 b_{32},$$

$$b_4 = Z_1 b_{41} + Z_2 b_{42}$$

$$\begin{aligned} \text{Dr} = & -(\alpha_2 \cosh(\alpha_2) + \beta_2 \sinh(\alpha_2)) \\ & * (\alpha_1 \sinh(\alpha_1) + \beta_1 \cosh(\alpha_1)) \\ & - \frac{\alpha_2 D}{\alpha_1} (\alpha_1 \cosh(\alpha_1) + \beta_1 \sinh(\alpha_1)) \\ & * (\alpha_2 \sinh(\alpha_2) + \beta_2 \cosh(\alpha_2)) \end{aligned}$$

$$g_1 = -l_3 (\alpha_1 \sinh(\alpha_1) + \beta_1 \cosh(\alpha_1)) * (\alpha_2 \sinh(\alpha_2) + \beta_2 \cosh(\alpha_2))$$

$$g_2 = \frac{l_2}{\alpha_1} (\alpha_1 \cosh(\alpha_1) + \beta_1 \sinh(\alpha_1)) * (\alpha_2 \sinh(\alpha_2) + \beta_2 \cosh(\alpha_2))$$

$$g_3 = -(l_2 - 2l_1 - \beta_1 (l_1 - l_2 + l_3)) * (\alpha_2 \sinh(\alpha_2) + \beta_2 \cosh(\alpha_2))$$

$$g_4 = -l_6 (\alpha_1 \sinh(\alpha_1) + \beta_1 \cosh(\alpha_1)) * (\alpha_2 \sinh(\alpha_2) + \beta_2 \cosh(\alpha_2))$$

$$g_5 = -\frac{D l_5}{\alpha_1} (\alpha_1 \cosh(\alpha_1) + \beta_1 \sinh(\alpha_1)) * (\alpha_2 \sinh(\alpha_2) + \beta_2 \cosh(\alpha_2))$$

$$g_6 = -(l_5 + 2l_4 + \beta_2 (l_4 + l_5 + l_6)) * (\alpha_1 \sinh(\alpha_1) + \beta_1 \cosh(\alpha_1))$$

$$b_{41} = \frac{-1}{\text{Dr}} (g_1 + g_2 + g_3), \quad b_{42} = \frac{-1}{\text{Dr}} (g_4 + g_5 + g_6),$$

$$b_{31} = \frac{-b_{41} (\alpha_2 \cosh(\alpha_2) + \beta_2 \sinh(\alpha_2))}{\alpha_2 \sinh(\alpha_2) + \beta_2 \cosh(\alpha_2)},$$

$$g_7 = -b_{42} (\alpha_2 \cosh(\alpha_2) + \beta_2 \sinh(\alpha_2)),$$

$$g_8 = -2l_4 - l_5 - \beta_2 (l_4 + l_5 + l_6),$$

$$g_{10} = 2l_1 - l_2 + \beta_1 (l_1 - l_2 + l_3),$$

$$b_{32} = \frac{g_7 + g_8}{\alpha_2 \sinh(\alpha_2) + \beta_2 \cosh(\alpha_2)}$$

$$b_{11} = b_{31} - l_3, \quad b_{12} = b_{32} + l_6$$

$$g_9 = b_{11} (\alpha_1 \sinh(\alpha_1) + \beta_1 \cosh(\alpha_1)),$$

$$b_{21} = \frac{g_9 + g_{10}}{\alpha_1 \cosh(\alpha_1) + \beta_1 \sinh(\alpha_1)},$$

$$b_{22} = \frac{b_{12} (\alpha_1 \sinh(\alpha_1) + \beta_1 \cosh(\alpha_1))}{\alpha_1 \cosh(\alpha_1) + \beta_1 \sinh(\alpha_1)}.$$

Case 2: Diffusion with Combined Homogeneous and Heterogeneous Chemical Reaction (One Fluid Model)

$$u = \frac{-p(1-\eta^2)}{2}, \quad \bar{u} = -\frac{p}{3}, \quad u_x = \frac{p\eta}{2} - \frac{p}{6},$$

$$A = \frac{p}{\alpha^3 \sinh(\alpha)}, \quad D^* = \frac{h^2 p^2}{D} F(\alpha)$$