

HOMOGENEOUS AND HETEROGENEOUS REACTIONS ON THE DISPERSION OF A SOLUTE IN A POROUS MEDIUM

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The effects of homogeneous and heterogeneous reactions on the dispersion of a solute in a porous medium in a magnetohydrodynamic laminar flow between two parallel plates is studied. In the case of diffusion with a first order homogeneous reaction, the effective dispersion coefficient increases with increase in the permeability of the porous medium, while it decreases with increase in Hartmann number. But in the case of diffusion combined with homogeneous and heterogeneous chemical reactions, permeability again increases the effective dispersion coefficient while increase in Hartmann number causes a decrease. The above analysis reveals that permeability of the medium promotes the rate of diffusion.

INTRODUCTION

The dispersion of soluble matter in an incompressible viscous fluid flowing in a circular pipe has been discussed by Taylor (1953, 1954a, 1954b) wherein it is observed that the solute is dispersed with an apparent diffusion coefficient $R^2 U_a^2 / 48D$, where R is the radius of the pipe, and U_a and D are the average velocity and molecular diffusion coefficient, respectively. Recently, Aris (1956) extended the above analysis with fewer departures from Taylor. The work was later extended to include dispersion in a non-Newtonian fluid also by Fan and Hwang (1965).

However, the above investigations do not take into account the chemical reaction of a solute during the process of dispersion in a solvent. We see a wide variety of situations in chemical engineering wherein diffusion of a solute takes place with simultaneous chemical reaction, namely, hydrolysis, gas absorption in an agitated tank, and ester experiments (Bird *et al.* 1960). The combined first order heterogeneous and homogeneous reactions on the dispersion of a solute have been studied by Walker (1961) and Solomon and Hudson (1967).

All the above investigations are, however, carried out to chemical reactions under steady state conditions until recently when Gupta and Gupta (1972) discussed for the unsteady case. They have analyzed the unsteady dispersion of solute with simultaneous chemical reaction in a liquid flowing in a channel by adopting Taylor's method. 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 and Krishna Murthy (1974). They found that the solute in an electrically conducting solvent can regulate rate of diffusion.

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However, the diffusion process, combined with homogeneous and heterogeneous chemical reactions of a solute in a porous medium, is also important in chemical engineering. The diffusion inside the tortuous void passages in the medium is pointed out by Bird *et al.* (1960, p. 542–46). They also pointed out that such study is important in a porous catalyst pellet, which is used in fixed-bed, axial-flow reactors. They described the “average” diffusion of the chemical species in terms of an effective diffusion co-efficient both for spherical porous catalyst and for non-spherical catalyst particles.

The present motivation comes from a desire to understand, at least qualitatively, the effect of porosity and its role in the dispersion of a solute in the presence of homogeneous and heterogeneous chemical reaction—in particular, to study the diffusion of a solute in a conducting solvent through a porous medium, which is undergoing a first order irreversible chemical reaction.

DIFFUSION WITH A HOMOGENEOUS FIRST-ORDER REACTION

We consider the dispersion of a solute in the laminar flow of a viscous conducting fluid through the porous medium between two parallel plates, distance $2d$ apart, under a uniform pressure gradient. The walls are assumed to be non-conducting and impermeable, x -axis being taken along the flow direction and y -axis being perpendicular to the walls. With applied uniform magnetic field along the y -axis, the velocity distribution (in non-dimensional form), as derived by Narasimha Murthy *et al.* (1972), is

$$u(\eta) = \frac{1}{\frac{1}{K} + M^2} \left[1 - \frac{\cosh \sqrt{\frac{1}{K} + M^2} \eta}{\cosh \sqrt{\frac{1}{K} + M^2}} \right], \quad \dots(1)$$

where $\eta = \frac{y}{\alpha}$, $M = \frac{\sigma}{\mu} B_0^2 d^2$ is Hartmann number and K is the permeability of the porous medium.

The average velocity is given by

$$\bar{u} = \frac{1}{\frac{1}{K} + M^2} \left[1 - \frac{\tanh \sqrt{\frac{1}{K} + M^2}}{\sqrt{\frac{1}{K} + M^2}} \right] \quad \dots(2)$$

If a solute diffuses in the fully developed flow as above, and simultaneously undergoes a first order irreversible chemical reaction under isothermal conditions, then the concentration equation for C is

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) - K_1 C, \quad \dots(3)$$

where D is the molecular diffusion coefficient and K_1 is the first-order reaction rate.

We now consider convection across a plane moving with the mean speed of the

flow. The velocity of the fluid relative to this plane is given by

$$u_x = u - \bar{u}$$

$$= \frac{1}{\frac{1}{K} + M^2} \left[\frac{\tan h \sqrt{\frac{1}{K} + M^2}}{\sqrt{\frac{1}{K} + M^2}} - \frac{\cos h \sqrt{\frac{1}{K} + M^2} \eta}{\cos h \sqrt{\frac{1}{K} + M^2}} \right] \quad \dots(4)$$

on assuming

$$\frac{\partial^2 C}{\partial x^2} \ll \frac{\partial^2 C}{\partial y^2}$$

and introducing the following dimensionless quantities

$$\theta = \frac{t}{\bar{t}}, \bar{t} = \frac{L}{\bar{u}}, \xi = \frac{x - \bar{u}t}{L}, \eta = \frac{y}{d} \quad \dots(5)$$

and using Taylor's limiting condition, we obtain Eq. (3) as

$$-K_1 \frac{d^2}{D} C + \frac{\partial^2 C}{\partial \eta^2} = \frac{d^2 u_x}{DL} \frac{\partial C}{\partial \xi} \quad \dots(6)$$

Using Eq. (4) in Eq. (6) and integrating, using the boundary conditions

$$\frac{\partial C}{\partial \eta} = 0 \text{ at } \eta = 1, \frac{\partial C}{\partial \eta} = 0 \text{ at } \eta = 0, \quad \dots(7)$$

we obtain for concentration

$$C = A \cos h \alpha \eta + \frac{d^2}{\alpha DL (1/K + M^2)} \cdot \frac{\partial C}{\partial \xi} \left[\frac{\alpha \cos h \sqrt{\frac{1}{K} + M^2} \eta}{\cos h \sqrt{\frac{1}{K} + M^2} \left\{ \alpha^2 - \left(\frac{1}{K} + M^2 \right) \right\}} - \frac{\tan h \sqrt{\frac{1}{K} + M^2}}{\alpha \sqrt{\frac{1}{K} + M^2}} \right] \quad \dots(8)$$

where

$$A = \frac{d^2 (\partial C / \partial \xi)}{DL \left(\frac{1}{K} + M^2 \right) \sin h \alpha} \cdot \frac{\tan h \sqrt{\frac{1}{K} + M^2}}{\sqrt{\frac{1}{K} + M^2}} \quad \dots(9)$$

and

$$\alpha = d \left(\frac{K_1}{D} \right)^{\frac{1}{2}}, \quad \dots(10)$$

which is the homogeneous reaction rate parameter.

The first boundary condition in the above expresses zero mass transport at the walls, while the second follows from the symmetry of the concentration profile about the central line of the channel.

The volumetric rate at which the transportation of the solute takes place across a section of the channel of unit breadth is

$$Q = \int_{-1}^1 C u_x d\eta. \quad \dots(11)$$

Using Eqs. (4) and (8), we obtain

$$Q = \frac{2d^4 (\partial c / \partial \xi) K_1 L^2}{\left(\frac{1}{K} + M^2\right) \cdot D^2 L^3 2\alpha^3} \left[\frac{2 \tan^2 h \sqrt{\frac{1}{K} + M^2}}{\alpha \left(\frac{1}{K} + M^2\right)} \right. \\ + \frac{\sqrt{\frac{1}{K} + M^2} \cdot \tan h \sqrt{\frac{1}{K} + M^2}}{\sin h \alpha \cdot \left\{ \alpha^2 - \left(\frac{1}{K} + M^2\right) \right\} \cos h \sqrt{\frac{1}{K} + M^2}} \left. \left\{ \frac{\sin h \left(\alpha + \sqrt{\frac{1}{K} + M^2} \right)}{\alpha + \sqrt{\frac{1}{K} + M^2}} \right. \right. \\ + \left. \left. \frac{\sin h \left(\alpha - \sqrt{\frac{1}{K} + M^2} \right)}{\left(\alpha - \sqrt{\frac{1}{K} + M^2} \right)} \right\} \right] \frac{\alpha}{\left\{ \alpha^2 - \left(\frac{1}{K} + M^2\right) \right\} \cos^2 h \sqrt{\frac{1}{K} + M^2}} \\ \left[1 + \frac{\sin h 2\sqrt{\frac{1}{K} + M^2}}{2\sqrt{\frac{1}{K} + M^2}} \right] \quad \dots(12)$$

Comparing the above expression 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

$$D^* = \frac{d^4 K_1 L^2}{D^2 \left(\frac{1}{K} + M^2\right)} F(\alpha) \quad \dots(13)$$

where

$$F(\alpha) = \frac{1}{\alpha^3} \left[\frac{2 \tan^2 h \sqrt{\frac{1}{K} + M^2}}{\alpha \left(\frac{1}{K} + M^2\right)} + \frac{\sqrt{\frac{1}{K} + M^2} \tan h \sqrt{\frac{1}{K} + M^2}}{\left\{ \alpha^2 - \left(\frac{1}{K} + M^2\right) \right\} \sin h \alpha \cos h \sqrt{\frac{1}{K} + M^2}} \right]$$

$$\left\{ \frac{\sinh\left(\alpha + \sqrt{\frac{1}{K} + M^2}\right)}{\alpha + \sqrt{\frac{1}{K} + M^2}} + \frac{\sinh\left(\alpha - \sqrt{\frac{1}{K} + M^2}\right)}{\alpha - \sqrt{\frac{1}{K} + M^2}} \right\} \frac{\alpha}{\left\{ \alpha^2 - \left(\frac{1}{K} + M^2\right) \right\} \cos^2 h \sqrt{\frac{1}{K} + M^2}} \left\{ 1 + \frac{\sinh 2\sqrt{\frac{1}{K} + M^2}}{2\sqrt{\frac{1}{K} + M^2}} \right\} \dots (14)$$

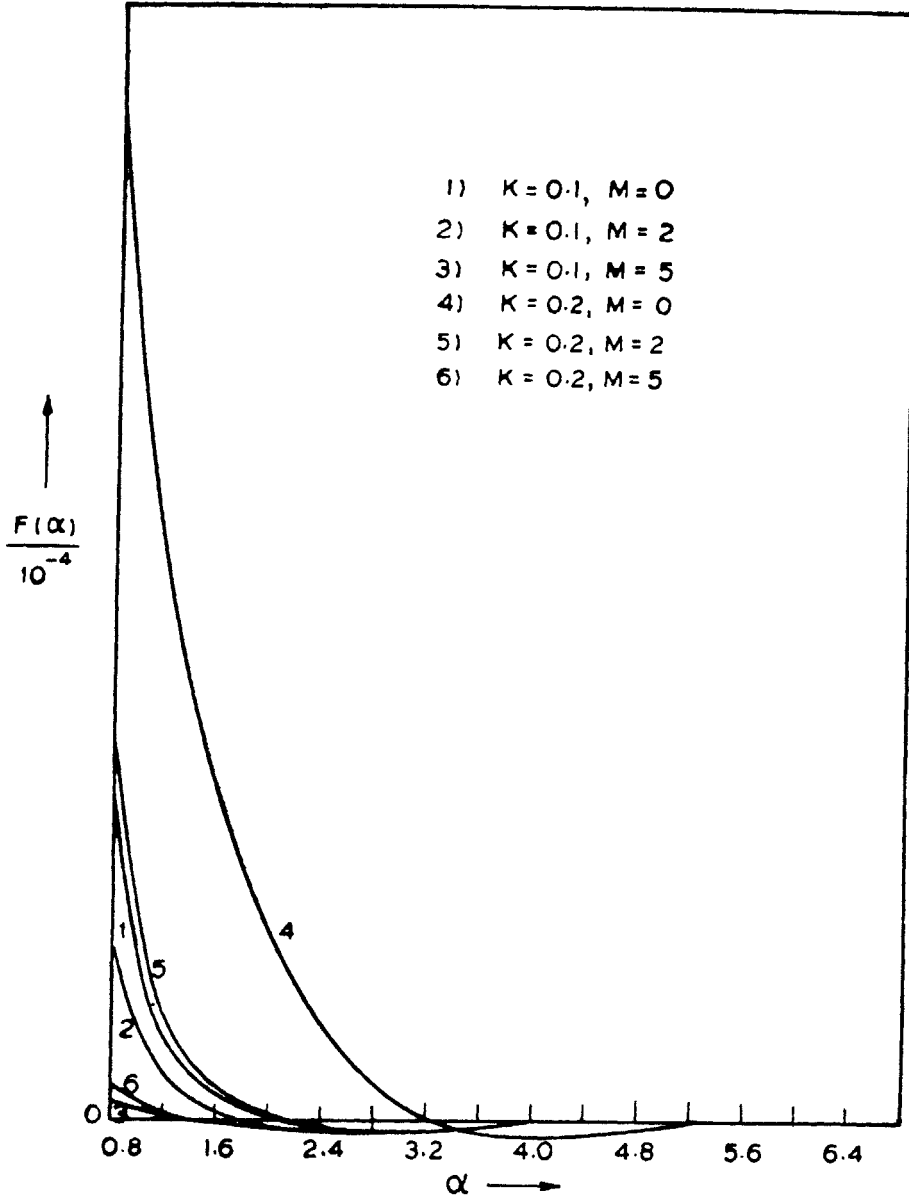


FIG. 1

The values of D^* versus α , the reaction rate parameter, for various values of the permeability and Hartmann number are plotted in Fig. 1. We observe that the effective dispersion coefficient decreases with increase in reaction rate for a fixed value of the permeability and Hartmann number. With increase in Hartmann number, the effective dispersion coefficient decreases for a fixed value of permeability. Further, for a fixed value of Hartmann number, the effective dispersion coefficient increases with increase in permeability. This is expected as can be seen from expression (14) that D^* is directly proportional to K . In other words, the increase in permeability leads to the decrease in the number of moles of solute undergoing chemical reaction resulting in increase in effective dispersion coefficient. The result that the dispersion coefficient decreases with increase in Hartmann number and the reaction rate is in conformity with our Narasimha Murthy and Krishnamurthy (1974) earlier result. When $K \rightarrow 0$, we recover our (Narasimha Murthy & Krishnamurthy 1974) result.

DIFFUSION WITH COMBINED HOMOGENEOUS AND HETEROGENEOUS REACTION

From what follows, we discuss the problem of diffusion in a channel with first order irreversible chemical reaction taking place both in the bulk of the medium and at the walls of the channel, which are assumed to be catalytic to reaction and non-conducting to electromagnetic effects.

In this case, the diffusion equation

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial y^2} - K_1 C \quad \dots(15)$$

is to be solved with the following boundary conditions

$$\begin{aligned} \frac{\partial C}{\partial y} + fC &= 0 & \text{at } y = d \\ \frac{\partial C}{\partial y} - fC &= 0 & \text{at } y = -d \end{aligned} \quad \dots(16)$$

Again, introducing the dimensionless quantities as in Eq. (5), and assuming limiting conditions of Taylor, the diffusion equation to be solved now is

$$-K_1 \frac{d^2}{D} C + \frac{\partial^2 C}{\partial \eta^2} = \frac{d^2}{DL} u_x \frac{\partial C}{\partial \xi} \quad \dots(17)$$

with boundary conditions

$$\begin{aligned} \frac{\partial C}{\partial \eta} + \beta C &= 0 & \text{at } \eta = 1, \\ \frac{\partial C}{\partial \eta} - \beta C &= 0 & \text{at } \eta = -1, \end{aligned} \quad \dots(18)$$

where $\beta = fd$, which is the heterogeneous reaction rate parameter which corresponds to catalytic reaction at the walls.

The solution of Eq. (17), subjected to boundary conditions (18), is

$$C = \frac{d^2}{DL\left(\frac{1}{K} + M^2\right)} \frac{\partial C}{\partial \xi} \left[\frac{\beta \tan h \sqrt{\frac{1}{K} + M^2}}{\alpha \sqrt{\frac{1}{K} + M^2}} - \frac{\alpha \beta}{\alpha^2 - \left(\frac{1}{K} + M^2\right)} \right. \\ \left. - \frac{\alpha \sqrt{\frac{1}{K} + M^2} \tanh \sqrt{\frac{1}{K} + M^2}}{\alpha^2 - \left(\frac{1}{K} + M^2\right)} \cos h \alpha \eta + \frac{\alpha \cos h \left(\sqrt{\frac{1}{K} + M^2}\right) \eta}{\left\{ \alpha^2 - \left(\frac{1}{K} + M^2\right) \right\} \cos h \sqrt{\frac{1}{K} + M^2}} \right. \\ \left. \frac{\tan h \sqrt{\frac{1}{K} + M^2}}{\alpha \sqrt{\frac{1}{K} + M^2}} \right] \dots (19)$$

Again, the volumetric rate at which the solute is transported across a section of the channel of unit breadth is

$$Q = \int_{-1}^1 C u_x d\eta \dots (20)$$

Again substituting Eq. (19) and Equation (4), we obtain

$$Q = \frac{2d^4 \left(\frac{\partial C}{\partial \xi}\right) K_1 L^2}{\left(\frac{1}{K} + M^2\right)^2 D^2 L^3} \frac{1}{2\alpha^3} \left[\frac{1}{\alpha \sin h \alpha + \beta \cos h \alpha} \right. \\ \left. \left\{ \frac{\beta \tan h \sqrt{\frac{1}{K} + M^2}}{\alpha \sqrt{\frac{1}{K} + M^2}} - \frac{\alpha \beta}{\alpha^2 - \left(\frac{1}{K} + M^2\right)} - \frac{\alpha \sqrt{\frac{1}{K} + M^2} \tan h \sqrt{\frac{1}{K} + M^2}}{\alpha^2 - \left(\frac{1}{K} + M^2\right)} \right\} \right. \\ \left. \left\{ \frac{12 \tan h \sqrt{\frac{1}{K} + M^2}}{\alpha \sqrt{\frac{1}{K} + M^2}} \frac{\sin h \alpha}{\alpha} - \frac{1}{\cos^2 h \sqrt{\frac{1}{K} + M^2}} \left(\frac{\sinh \left(\alpha + \sqrt{\frac{1}{K} + M^2}\right)}{\alpha + \sqrt{\frac{1}{K} + M^2}} \right) \right\} \right]$$

$$\left. \frac{\sin h \left(\alpha - \sqrt{\frac{1}{K} + M^2} \right)}{\alpha - \sqrt{\frac{1}{K} + M^2}} \right\} + \frac{2 \alpha \tan h^2 \sqrt{\frac{1}{K} + M^2}}{\left(\frac{1}{K} + M^2 \right) \left\{ \alpha^2 - \left(\frac{1}{K} + M^2 \right) \right\}}$$

$$\frac{\alpha}{\left\{ \alpha^2 - \left(\frac{1}{K} + M^2 \right) \right\} \cos^2 h \sqrt{\frac{1}{K} + M^2}} \left(1 + \frac{\sin h 2 \sqrt{\frac{1}{K} + M^2}}{2 \sqrt{\frac{1}{K} + M^2}} \right) \dots (21)$$

Comparing (21) with Fick's law diffusion, we find that the solute is dispersed relative to a plane moving with the mean speed of the flow with an effective dispersion co-efficient D^* given by

$$D^* = \frac{d^4 K_1 L^2}{2 D^2} G(\alpha, \beta) \dots (22)$$

where

$$G(\alpha, \beta) = \frac{1}{\alpha^3 \left(\frac{1}{K} + M^2 \right)^2} \left[\frac{1}{\alpha \sin h \alpha + \beta \cosh \alpha} \left\{ \frac{\beta \tan h \sqrt{\frac{1}{K} + M^2}}{\alpha \sqrt{\frac{1}{K} + M^2}} - \frac{\alpha \beta}{\alpha^2 - \left(\frac{1}{K} + M^2 \right)} \frac{\alpha \sqrt{\frac{1}{K} + M^2} \tan h \sqrt{\frac{1}{K} + M^2}}{\alpha^2 - \left(\frac{1}{K} + M^2 \right)} \right\} \left\{ \frac{2 \tan h \sqrt{\frac{1}{K} + M^2}}{\alpha \sqrt{\frac{1}{K} + M^2}} \right. \right.$$

$$\left. \left. \frac{\sin h \alpha}{\alpha} - \frac{1}{\cos^2 h \sqrt{\frac{1}{K} + M^2}} \left(\frac{\sin h \left(\alpha + \sqrt{\frac{1}{K} + M^2} \right)}{\alpha + \sqrt{\frac{1}{K} + M^2}} + \frac{\sin h \left(\alpha - \sqrt{\frac{1}{K} + M^2} \right)}{\alpha - \sqrt{\frac{1}{K} + M^2}} \right) \right\} \right.$$

$$\left. + \frac{2 \alpha \tan h^2 \sqrt{\frac{1}{K} + M^2}}{\left(\frac{1}{K} + M^2 \right) \left\{ \alpha^2 - \left(\frac{1}{K} + M^2 \right) \right\}} - \frac{\alpha}{\left\{ \alpha^2 - \left(\frac{1}{K} + M^2 \right) \right\} \cos^2 h \sqrt{\frac{1}{K} + M^2}} \left(1 + \frac{\sin h 2 \sqrt{\frac{1}{K} + M^2}}{2 \sqrt{\frac{1}{K} + M^2}} \right) \right] \dots (23)$$

When $K = 0$, we recover our (Narasimha Murthy & Krishnamurthy 1974) earlier result. The values of $G(\alpha, \beta)$ for various values of β and different sets of values

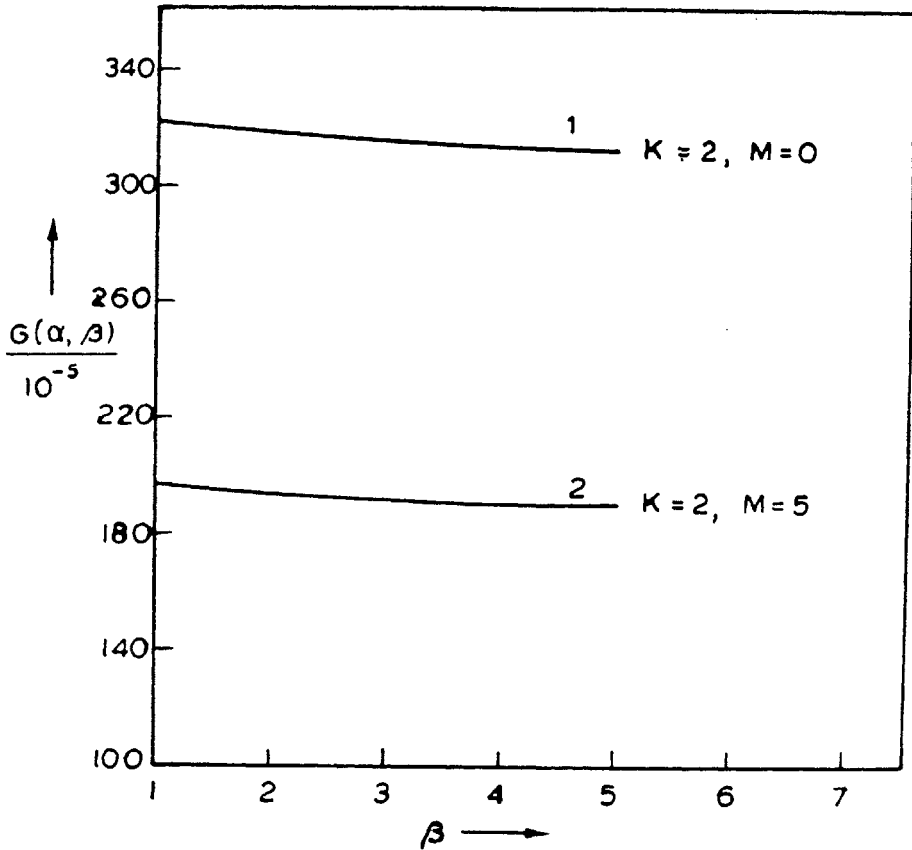


FIG. 2

of K and M , the permeability and Hartmann number are computed. This is shown in Fig. 2. Also, in this case, the increase in the wall catalytic parameter together with Hartmann number causes a decrease in the effective dispersion coefficient for a fixed value of permeability. On the other hand, increase in permeability causes an increase in the effective dispersion coefficient.

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