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ABSTRACT

Title of Thesis : Dispersion in the Laminar Flow of Ellis
Model Fluids Through Straight Tubes

Yeong-Hua Huang, Master of Science, 1986

Thesis directed by : Dr. Wing T. Wong

Taylor-Aris dispersion theory is extended to the laminar tube flow of Carreau model fluids and Ellis model fluids and the results are compared with those of power law fluids. It is found that Carreau and Ellis models are more appropriate than power-law model, especially at low pressure gradient.

An exact solution to the unsteady convective diffusion equation in fully developed laminar flow in tube is obtained by applying the generalized dispersion theory of Gill and Sankarasubramanian for Ellis model. The results are compared with those obtained by Booras and Krantz for power-law model. The most interesting result of this work is that the power law is valid only at high shear stress, whereas Ellis model allows the prediction of dispersion coefficient and mean solute distribution over much wider range of external pressure gradient.

Dispersion in the Laminar Flow of Ellis Model

Fluids Through Straight Tubes.

BY

YEONG-HUA HUANG

Thesis submitted to the Faculty of the Graduate School
of the New Jersey Institute of Technology in partial
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I. INTRODUCTION

Over the past 20 years the public has been justifiably concerned with the protection of environment. In some cases, chemicals like pesticides and perfumes are deliberately released; in other cases, chemicals like hydrogen sulfide can be accidentally spilled. In all cases, the public worries about the long-term effects of such chemical pollutions.

Public concern has led to legislations at federal, state, and local levels. These legislations usually are phased in terms of regulations of chemical concentrations. These regulations take different forms. The maximum allowable concentration may be averaged over a day or over a year. The acid concentration (as pH) can be held within a particular range, or the number and size of particles going up a stack can be restricted. Those working with chemicals must be able to anticipate whether or not these chemicals can be adequately dispersed.

As might be expected, dispersion is related to diffusion. Diffusion is a molecular process governed by laws of thermodynamics, whereas dispersion is the combined effect of diffusion and convection. The relation exists on two very different levels. First, dispersion is a form of mixing, and so on a microscopic scale it involves diffusion of molecules. This microscopic dispersion is not understood in detail, but it takes place so rapidly that it is rarely the most important feature of the process. Second, dispersion and

diffusion are described with very similar mathematics. This means that analyses developed for diffusion can often correlate results for dispersion.

Dispersion theory is concerned with the dispersal of a solute in a flowing fluid due to the combined action of a nonuniform velocity profile, molecular diffusion, and eddy diffusion in the case of turbulent flow. Numerous papers have discussed dispersion in a variety of laminar and turbulent flows since Sir Geoffrey Taylor (1953) and Aris (1956) published the first papers on the subject.

Developments in the areas of polymer processing, biomedical engineering, and biochemical processing have contributed to the ever-increasing interests in the flow and properties of non-Newtonian fluids. Typical occurrences of this dispersion phenomenon in applications involving non-Newtonian fluids include the behavior of dyes in injection molding process, the determination of the residence time of tracer solutes injected into the bloodstream, and the transport of slurries and polymer solutions.

However, most papers have been focused on dispersion in Newtonian fluids. Relatively few papers have considered dispersion in non-Newtonian fluids. Taylor-Aris dispersion theory had been extended to the laminar flow of power-law, Bingham plastic, and Ellis fluids in circular tube by Fan and co-workers (1965,1966). Ananthakrishnan et al. (1965) have

shown that Taylor-Aris dispersion theory for Newtonian fluids applies only for sufficiently large values of the dimensionless time $\tau (=Dt/R^2)$ ranging from 0.80 at $Pe=500$ to 20 at $Pe=1$. This limitation of Taylor-Aris dispersion theory led Gill (1967) and Gill and Sankertasubramanian (1970) to develop a generalized dispersion theory for unsteady convective diffusion in Newtonian fluids which is valid for all values of τ and which reduces to Taylor-Aris results for large values of τ . Gill and co-workers (Gill and Sankarasubramanian (1971,1972) ; Sankarasubramanian and Gill (1972,1973)) have extended this analysis to non-uniformly distributed and time-variable sources as well as to time variable laminar flows including mass transfer at the tube wall. Indeed, the generalized dispersion theory of Gill and co-workers has permitted us to consider dispersion phenomena in a wide variety of flow scenarios which hitherto were far too complex to solve analytically.

In order to understand more fully the rather limited domain of Taylor-Aris dispersion theory, let us estimate the transit time T or equivalently the tube length L necessary for Taylor-Aris theory to apply, assuming a typical liquid phase diffusivity of $10^{-5} \text{ cm}^2/\text{s}$ and $Pe=500$. Then, according to the criterion obtained by Ananthakrishnan et al., $T > 8\text{s}$ and $L > 4\text{cm}$ for $R=0.01\text{cm}$; $T > 800\text{s}$ and $L > 40\text{cm}$ for $R=1\text{cm}$; and $T > 80000\text{s}$ and $L > 400\text{cm}$ for $R=1\text{cm}$. However, many dispersion phenomena of practical interest occur for time period $\tau < 0.8$ and thus are

more properly described by the generalized dispersion analysis of Gill and co-workers than by Taylor-Aris theory.

Clearly, it is desirable to apply the generalized dispersion theory of Gill and co-workers to the dispersion process in non-Newtonian fluids as was done by Booras and Krantz (1976) for power-law fluids.

In the present study, Ellis model is applied to the generalized dispersion theory instead of the power-law model, since it is a flexible empirical model, which includes the Newtonian regime at low shear rate and the power-law at high shear rate. We know that power-law model is not applicable for pipe flow, because by symmetry the shear rate is zero at the axis and hence the power-law model would imply an infinite viscosity for shear-thinning fluid. This property of power-law model implies some limitations in the application of generalized dispersion theory.

Before we apply the generalized dispersion theory approach of Gill and co-workers to the dispersion process in Ellis model fluids, we have considered the Taylor-Aris dispersion theory of the laminar tube flow of Carreau model fluids, and compared the results with those obtained for power-law and Ellis fluids. From the results of these three models, it may be concluded that in applying the generalized dispersion theory the three-parameter Ellis model is more appropriate than the two-parameter power-law model.

II. THEORY

A. Dispersion in the laminar flow of a Carreau fluid through straight circular tube

In a series of papers, Taylor (1953,1954a,b) treated the problem of dispersion of a soluble tracer in a solvent flowing in a circular pipe. His results have been generally confirmed by experiments. However it should be noted that Taylor's work was only concerned with Newtonian fluids, Fan and co-worker applied Taylor's theory to power-law, Bingham and Ellis fluids. In this section the dispersion of a tracer material in the laminar tube flow of a fluid, described by the Carreau model, is discussed using the Taylor-Aris dispersion theory .

In a cylindrical tube, the variation of tracer concentration, C , as a function of time, t , radial position, r , and axial distance along the tube, x , may be expressed by the following partial differential equation

$$\frac{\partial C}{\partial t} = D \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C}{\partial r} \right) + \frac{\partial^2 C}{\partial x^2} \right] - V_x \frac{\partial C}{\partial x} \quad (1)$$

where D is the molecular diffusivity and $V_x(r)$ is the fully developed axial velocity as a function of radial position. When the molecular diffusivity is taken to be zero, only the convective term accounts for material transport. Otherwise, both the action of convection and radial material transport due to molecular diffusion will account for the dispersion

mechanisms.

1. Effect of Molecular Diffusion on the Fluid Dispersion

Equation (1) signifies that the distribution of tracer concentration in laminar flow is due to the combined action of convection along the tube induced by variation of velocity over the cross-section and radial dispersion caused by molecular diffusion.

In general, the transfer of C along tube by molecular diffusion is small compared with that produced by convection. It will be assumed therefore that $\partial^2 C / \partial x^2$ is small compared with

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C}{\partial r} \right) \quad \text{and} \quad v_x(r) \frac{\partial C}{\partial x}$$

The concentration and velocity will be defined relative to axes which move with the mean fluid velocity \bar{V}_x , that is

$$x_1 = x - \bar{V}_x t \quad (2)$$

We will see that the transformation to a frame of reference moving with the average velocity of the fluid is not simply for convenience, but rather it is a powerful tool to obtain an effective dispersion coefficient (K) which includes the combined action of convection and molecular dispersion.

Then equation (1) becomes

$$\frac{\partial C}{\partial t} = D \left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right) - (V_x(r) - \bar{V}_x) \frac{\partial C}{\partial x_1} \quad (3)$$

2. Carreau Model Fluids

The Carreau model, a four-parameter model which has been demonstrated to fit empirical data of many non-Newtonian fluids very well ([24]), can be expressed in terms of shear rate

$$\frac{\eta - \eta_{\infty}}{\eta_0 - \eta_{\infty}} = [1 + (\lambda \dot{\gamma})^2]^{\frac{n-1}{2}}$$

where η_0 is the zero-shear-rate viscosity, η_{∞} is the infinite-shear-rate viscosity, λ is a characteristic time and n is equivalent to the power-law index. This model may also be written in terms of shear stress as

$$\frac{\eta - \eta_{\infty}}{\eta_0 - \eta_{\infty}} = [1 + \left(\frac{\tau}{\tau_0} \right)^2]^{\frac{n-1}{2n}} \quad (4)$$

where τ_0 is a characteristic stress.

For polymer melt, η_{∞} is typically two to three orders of magnitude smaller than η_0 and so may be neglected. This means that

$$\frac{\eta}{\eta_0} = [1 + \left(\frac{\tau}{\tau_0} \right)^2]^{\frac{n-1}{2n}}$$

and

$$\dot{\gamma} = \frac{\tau}{\eta} = -\frac{dv_x}{dr} = \frac{\tau}{\eta_0 \left[1 + \left(\frac{\tau}{\tau_0} \right)^2 \right]^{\frac{n-1}{2n}}} \quad (5)$$

$$dv_x = - \frac{\tau}{\eta_0 \left[1 + \left(\frac{\tau}{\tau_0} \right)^2 \right]^{\frac{n-1}{2n}}} dr$$

From the equations of motion, the momentum flux distribution in cylindrical tube is found to be

$$\tau_{rx} = \frac{\Delta P}{2L} r \quad (6)$$

where ΔP is the pressure drop over a tube length L .

Equation (5) is simplified by setting $\xi = r/R$ and letting

$$a = \frac{\Delta P R^2}{2\eta_0 L} \quad (7a)$$

and

$$b = \frac{\Delta P R}{2\tau_0 L} \quad (7b)$$

Then integration of equation (5) with the no-slip boundary condition yields the isothermal and steady-state velocity profile

$$V_x(\xi) = \frac{an}{n+1} b^{\frac{1-n}{n}} \left[(b^{-2}+1)^{\frac{n+1}{2n}} - (b^{-2} + \xi^2)^{\frac{n+1}{2n}} \right] \quad (8)$$

and

$$\bar{V}_x = 2 \int_0^1 \xi V_x d\xi \quad (9)$$

Substituting (7) and (8) into (9) gives

$$V_x = \frac{an}{n+1} b^{\frac{n-1}{n}} (b^{-2}+1)^{\frac{n+1}{2n}} - \frac{2an}{(n+1)(3n+1)} b^{\frac{1-n}{n}} \left[(b^{-2}+1)^{\frac{3n+1}{2n}} - b^{\frac{3n+1}{n}} \right] \quad (10)$$

Normalizing (3) by introducing the dimensionless variables C^* , Θ , ξ , and η_1 , we obtain

$$\frac{\partial C^*}{\partial \Theta} = \frac{D \underline{t}}{R^2} \left(\frac{\partial^2 C^*}{\partial \xi^2} + \frac{1}{\xi} \frac{\partial C^*}{\partial \xi} \right) - \frac{1}{\bar{V}_x} [V_x - \bar{V}_x] \frac{\partial C^*}{\partial \eta_1} \quad (11)$$

where

C^* = dimensionless concentration = C/C_0

Θ = dimensionless time = $t/\underline{t} = t\bar{V}_x/L$

ξ = dimensionless radial distance = r/R

\underline{X} = dimensionless axial distance = x/L

$\eta_1 = \underline{X} - \Theta$

Here $\partial/\partial\Theta$ represents differentiation with respect to time at a point fixed relative to axes moving with the mean velocity. Since the moving axes have been introduced, the transfer of tracer concentration across plane at which η_1 is constant

depends only on the radial variation of tracer concentration because the mean velocity across such planes is zero. It is further assumed (Taylor, 1953) that the time necessary for appreciable effects to appear, owing to convective transport, is long compared with the 'time of decay' during which radial variations of concentration are reduced to a fraction of their initial value through the action of molecular diffusion, which means that the radial variation of tracer concentration is small, i.e., Taylor's limiting condition is satisfied, and thus $\partial C^*/\partial \theta$ is also small. Now we can approximately calculate the radial variation of C^* by first neglecting the $\partial C^*/\partial \theta$ term

$$\frac{\partial^2 C^*}{\partial \xi^2} + \frac{1}{\xi} \frac{\partial C^*}{\partial \xi} = \frac{R^2}{D \bar{v}_x} [v_x - \bar{v}_x] \frac{\partial C^*}{\partial \eta_1} \quad (12)$$

In solving this equation $\partial C^*/\partial \eta_1$ may be taken as independent of ξ because moving coordinate is used. The boundary condition

$$\frac{\partial C^*}{\partial \xi} = 0 \quad \text{at } \xi = 1$$

is employed. The result for this case is

$$C^* = C_0 + \frac{R}{D \bar{v}_x} \left[\int_0^{\xi} \frac{d\xi''}{\xi''} \int_0^{\xi''} v_x \xi' d\xi' - \frac{\bar{v}_x}{4} \xi \right] \frac{\partial C^*}{\partial \eta_1} \quad (13)$$

where C_0 is the value of C^* at $\xi = 0$.

The rate of transport of C^* across a section at fixed η_1 is

$$Q = 2\pi R^2 \int_0^1 C^* (v_x - \bar{v}_x) \xi d\xi \quad (14)$$

Substituting (8), (10) and (13) into (14) and integrating over the range (0,1) and comparing this with Fick's law of diffusion, we find that an effective dispersion coefficient K can be defined

$$\begin{aligned} K = & -2 \frac{R^2}{D} \left(\frac{p^2}{16} - \frac{p\bar{v}_x}{8} + \frac{\bar{v}_x^2}{16} + \frac{nq}{4(3n+1)} (p - \bar{v}_x) \left[(b^{-2} + 1) \frac{3n+1}{2n} + b \frac{3n+1}{n} \right] \right. \\ & + \frac{n^2 q}{(3n+1)(5n+1)} (p - \bar{v}_x) \left[(b^{-2} + 1) \frac{3n+1}{2n} - b \frac{5n+1}{n} \right] \\ & + \left[\frac{n^2 q^2}{(3n+1)^2} (b^{-2} + 1) \frac{3n+1}{2n} - \frac{npq}{2(3n+1)} \right] \int_0^1 \left[\frac{(b^{-2} + \xi^2)}{\xi} - \frac{b}{\xi} - \frac{3n+1}{n} \right] d\xi \\ & - \frac{n^2 q^2}{(3n+1)^2} \int_0^1 \left[\frac{(b^{-2} + \xi^2)}{\xi} - b \frac{3n+1}{n} \frac{(b^{-2} + \xi^2)}{\xi} \right] d\xi \\ & \left. - \frac{nq\bar{v}_x}{2(3n+1)} \int_0^1 \left[\frac{(b^{-2} + \xi^2)}{\xi} - \frac{b}{\xi} - \frac{3n+1}{n} \right] d\xi \right) \\ = & -2 \frac{R^2}{D} K \end{aligned} \quad (15)$$

where

$$p = \frac{an}{n+1} b^{\frac{1-n}{n}} (b^{-2} + 1)^{\frac{n+1}{2n}} \quad (16a)$$

$$q = \frac{an}{n+1} b^{\frac{1-n}{n}} \quad (16b)$$

$$K \text{ stands for all the terms in the } () \quad (16c)$$

3. Ellis Model Fluids

The shear stress and viscosity relation of the Ellis model fluid is characterized by

$$\frac{\tau_0}{\eta} = 1 + \left(\frac{\tau_{rx}}{\tau_x} \right)^{\alpha-1} \quad (17)$$

in which τ_0 is the zero-shear-rate viscosity, τ_x is the value of the shear stress at which $\tau = \tau_0/2$, and $\alpha-1$ is the slope of $(\tau_0/\eta)-1$ vs. τ/τ_x on log-log paper.

$$\tau_{rx} = \eta \dot{\gamma} = \frac{\tau_0}{1 + \left(\frac{\tau_{rx}}{\tau_x} \right)^{\alpha-1}} \dot{\gamma}$$

$$\dot{\gamma} = -\frac{dV_x}{dr} = \frac{\tau_{rx}}{\tau_0} \left[1 + \left(\frac{\tau_{rx}}{\tau_x} \right)^{\alpha-1} \right] \quad (18)$$

and substituting (6) into (18), the velocity profile V_x is

given by

$$V_x = V_{m1}[1-\xi^2] + V_{m2}[1-\xi^{\alpha+1}] \quad (19)$$

where

$$V_{m1} = \frac{\Delta P R^2}{4\eta_0 L} \quad (20a)$$

$$V_{m2} = \frac{\tau_x R^{\alpha+1}}{\eta_0(\alpha+1)} \left(\frac{\Delta P}{2\tau_x L} \right)^\alpha \quad (20b)$$

from which the mean velocity can be readily obtained,

$$\bar{V}_x = \frac{1}{2}V_{m1} + \frac{\alpha+1}{\alpha+3}V_{m2} \quad (21)$$

Following the procedures in section 2 the effective dispersion coefficient K becomes

$$K = \frac{R^2}{D} \left[\frac{1}{192} V_{m1}^2 + \frac{(n+1)^2}{2(n+3)^3(n+5)} V_{m2}^2 + \frac{(n+1)(n+11)}{12(n+3)(n+5)(n+7)} V_{m1}V_{m2} \right] \quad (22)$$

which has been obtained by Fan and Wang (1965).

4. Power-law Model Fluids

$$\eta = m\dot{\gamma}^{n-1} \quad (23)$$

where m and the dimensionless quantity n are constants characteristic of the fluid. The velocity profile $V_x(r)$ in this case is

$$V_x(r) = V_R \left[1 - \left(\frac{r}{R} \right)^{\frac{n+1}{n}} \right] \quad (24)$$

where

$$V_R = \frac{n}{n+1} \left(\frac{R \Delta P}{2 \mu L} \right)^{\frac{1}{n}} R \quad (25)$$

and the mean velocity is

$$\bar{V}_x = \frac{n+1}{n+3} V_R \quad (26)$$

By analogous procedure as above, the effective dispersion coefficient K is determined to be

$$K = \frac{R^2}{D} \frac{\bar{V}_x^2}{2(n+3)(n+3)} \quad (27)$$

which has also been obtained by Fan and Hwang (1965).

5. Summary

From equations (15), (22), and (27) we have the effective dispersion coefficients, which were derived by applying the Taylor-Aris dispersion theory to Carreau model, Ellis model and power-law respectively.

Recall that (7a)

$$a = \frac{R \tau_R}{\tau_0} = Rg \quad (28)$$

we can rearrange equation (15) by taking (28) into equations (10), (16a) and (16b)

$$K = -2 \frac{R^4}{D} K' \quad (29)$$

$$\text{where } K' = \underline{K}/R^2$$

Equations (20a) and (20b) can also be arranged

$$V_{m1} = R \frac{\tau_R}{2\tau_0} = R \underline{V}_{m1} \quad (30a)$$

$$V_{m2} = R \frac{\tau_x}{\tau_0(\alpha+1)} \left(\frac{\tau_R}{\tau_x} \right)^\alpha = R \underline{V}_{m2} \quad (30b)$$

which lead (22) into

$$\frac{KD}{R^4} = \frac{1}{192} \underline{V}_{m1}^2 + \frac{(n+1)^2}{2(n+3)^3(n+5)} \underline{V}_{m2}^2 + \frac{(n+1)(n+11)}{12(n+3)(n+5)(n+7)} \underline{V}_{m1} \underline{V}_{m2} \quad (31)$$

(25) and (26) can be formed as

$$V_m = R \frac{n}{n+1} \left(\frac{\tau_R}{\tau_x} \right)^{\frac{1}{n}} = R \underline{V}_m \quad (32)$$

$$V_x = R \frac{n+1}{3n+1} \underline{V}_m \quad (33)$$

which lead (27) into

$$\frac{KD}{R^4} = \frac{(n+1)^2}{2(n+3)^3(n+5)} \underline{V}_m \quad (34)$$

B. Dispersion in the laminar flow of Ellis model fluids through straight tubes by the generalized dispersion theory approach of Gill and Sankarasubramanian

Purely convective dispersion creates infinite radial and axial concentration gradients. This physically unrealistic situation is in fact obviate by the action of radial and axial molecular diffusion. The former tends to reduce axial dispersion by reducing the radial concentration gradient, whereas the latter enhances axial dispersion by adding a purely diffusive axial component. A complete understanding of the action of molecular diffusion on the dispersion process demands a solution to the full unsteady-state convective diffusion equation which is given in equation (1).

For the slug input of solute of length x_s in a tube with radius R , the boundary conditions may be written as

$$C(0, x, r) = C_0 \quad (|x| \leq x_s) \quad (35a)$$

$$C(0, x, r) = 0 \quad (|x| > x_s) \quad (35b)$$

$$C(t, \infty, r) = 0 \quad (35c)$$

$$\frac{\partial C}{\partial r}(t, x, 0) = \frac{\partial C}{\partial r}(t, x, R) = 0 \quad (35d)$$

For Ellis model fluid, by applying (19) into (1) the equation of diffusion (1) can be re-written as

$$\frac{\partial C}{\partial t} (V_{m1} [1 - (\frac{r}{R})^2] + V_{m2} [1 - (\frac{r}{R})^{\alpha+1}]) = D \left[\frac{\partial^2 C}{\partial x^2} + \frac{1}{r} \frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial r^2} \right] \quad (36)$$

In dimensionless form, (35) and (36) become

$$\frac{\partial \theta}{\partial \tau} \frac{1}{V_0} [V_{m1}(1-y^2) + V_{m2}(1-y^{\alpha+1})] \frac{\partial \theta}{\partial X} = \frac{\partial^2 \theta}{\partial y^2} + \frac{1}{y} \frac{\partial \theta}{\partial y} + \frac{1}{Pe^2} \frac{\partial^2 \theta}{\partial X^2} \quad (37)$$

with the conditions

$$\theta(0, X, y) = 1 \quad |X| \leq X_s \quad (38a)$$

$$\theta(0, X, y) = 0 \quad |X| > X_s \quad (38b)$$

$$\theta(\tau, X, 0) = 0 \quad (38c)$$

$$\frac{\partial \theta}{\partial y}(\tau, X, 0) = \frac{\partial \theta}{\partial y}(\tau, X, 1) = 0 \quad (38d)$$

where

$$\theta = \frac{C}{C_0}, \quad X = \frac{Dx}{R^2 V_0}, \quad X_s = \frac{Dx_s}{R^2 V_0}, \quad \tau = \frac{Dt}{R^2}, \quad y = \frac{r}{R}, \quad Pe = \frac{RV_0}{D}$$

$$V_0 = \text{maximum velocity} = V_{m1} + V_{m2}$$

1. Purely Convective Dispersion

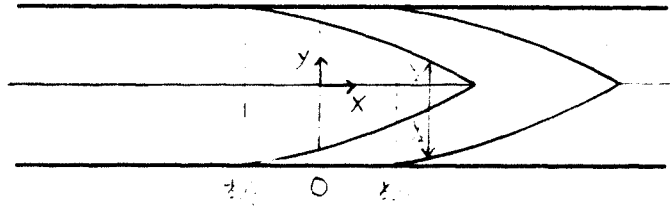
Let us consider the purely convective dispersion of an Ellis model fluid first.

$$\text{Since } X = V_x \tau$$

$$= \left[\frac{V_{m1}}{V_0} (1-y^2) + \frac{V_{m2}}{V_0} (1-y^{\alpha+1}) \right] \tau$$

$$\frac{X}{\tau} = 1 - \frac{V_{m1}}{V_0} y^2 - \frac{V_{m2}}{V_0} y^{\alpha+1} \quad (39)$$

For $\tau > X_s$, the mean concentration θ_m is given for purely convective dispersion by



$$\theta_n = 0 \quad (X < -\tau) \quad (40a)$$

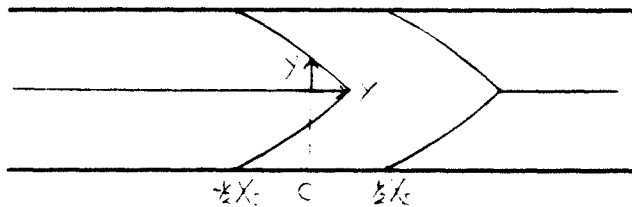
$$\theta_n = 1 - y^2 \quad (-\tau < X < 0) \quad (40b)$$

$$\theta_n = y_1^2 - y_2^2 \quad (0 < X < \tau) \quad (40c)$$

$$\theta_n = y^2 \quad (\tau < X < \tau + X_s) \quad (40d)$$

$$\theta_n = 0 \quad (\tau + X_s < X < \infty) \quad (40e)$$

and for $\tau < X_s$



$$\theta_n = 0 \quad (X < -\tau) \quad (41a)$$

$$\theta_n = 1 - y^2 \quad (-\tau < X < 0) \quad (41b)$$

$$\theta_n = 1 \quad (0 < X < \tau) \quad (41c)$$

$$\theta_n = y^2 \quad (\tau < X < \tau + X_s) \quad (41d)$$

$$\theta_n = 0 \quad (\tau + X_s < X < \infty) \quad (41e)$$

A plug of solute and a semi-infinite slug are special limiting cases of equation (40) and (41) for X_s being very small and very large, respectively.

2. Dispersion with Molecular Diffusion

Now let us consider the dispersion with molecular diffusion since we know that purely convective dispersion creates infinite radial and axial concentration gradients, and is physically unrealistic.

Define a new axial coordinate moving with the average velocity of flow as

$$x_1 = x - \bar{V}_x t$$

which in dimensionless form, is

$$X_1 = X - \frac{\tau}{V_0} \left(\frac{1}{2} v_{m1} + \frac{\alpha+1}{\alpha+3} v_{m2} \right) \quad (42)$$

$$V_{x1} = V_x - \bar{V}_x$$

$$= v_{m1} \left[\frac{1}{2} - y^2 \right] + v_{m2} \left[\frac{2}{\alpha+3} - y^{\alpha+1} \right] \quad (43)$$

so the governing diffusion equation (37) becomes

$$\frac{\partial \theta}{\partial \tau} + \frac{1}{V_0} \left[v_{m1} \left(\frac{1}{2} - y^2 \right) + v_{m2} \left(\frac{2}{\alpha+3} - y^{\alpha+1} \right) \right] \frac{\partial \theta}{\partial X_1} = \frac{\partial^2 \theta}{\partial y^2} + \frac{1}{y} \frac{\partial \theta}{\partial y} + \frac{1}{Pe^2} \frac{\partial^2 \theta}{\partial X_1^2} \quad (44)$$

Following the method of Gill and Sankarasubramanian (1970) we formulate the solution as a series expansion such that

$$\theta = \theta_m(\tau, X_1) + \sum_{k=1}^{\infty} f_k(\tau, y) \frac{\partial^k \theta_m}{\partial X_1^k} \quad (45)$$

where

$$\theta_n = 2 \int_0^1 y \theta dy \quad (46)$$

Upon substituting equation (45) into (44), the result is

$$\begin{aligned} & \frac{\partial}{\partial \tau} \left(\theta_n + \sum_{k=1}^{\infty} f_k \frac{\partial^k \theta_n}{\partial x_1^k} \right) + \frac{1}{V_0} \left(V_{n1} \left(\frac{1}{2} y^2 \right) + V_{n2} \left(\frac{2}{\alpha+3} y^{\alpha+1} \right) \right) \frac{\partial}{\partial x_1} \left(\theta_n + \sum_{k=1}^{\infty} f_k \frac{\partial^k \theta_n}{\partial x_1^k} \right) \\ &= \frac{1}{y} \frac{\partial}{\partial y} \frac{\partial}{\partial y} \left(\theta_n + \sum_{k=1}^{\infty} f_k \frac{\partial^k \theta_n}{\partial x_1^k} \right) + Pe^{-2} \frac{\partial^2}{\partial x_1^2} \left(\theta_n + \sum_{k=1}^{\infty} f_k \frac{\partial^k \theta_n}{\partial x_1^k} \right) \end{aligned} \quad (47)$$

Now if it is assumed that the process of distributing θ_n is diffusive in nature right from time zero one can write the generalized dispersion model in dimensionless form with time-dependent dispersion coefficients as

$$\frac{\partial \theta_n}{\partial \tau} = \sum_{i=1}^{\infty} K_i(\tau) \frac{\partial^i \theta_n}{\partial x_1^i} \quad (48)$$

It is important to note that K_i are a function of τ even though the velocity field is independent of τ .

Introducing equation (48) into (47) and rearranging terms,

$$\begin{aligned} & \sum_{i=1}^{\infty} K_i \frac{\partial^i \theta_n}{\partial x_1^i} + A \frac{\partial \theta_n}{\partial x_1} - Pe^{-2} \frac{\partial^2 \theta_n}{\partial x_1^2} \\ & + \sum_{k=1}^{\infty} \left(\left(\frac{\partial f_k}{\partial \tau} - \frac{1}{y} \frac{\partial f_k}{\partial y} \right) \frac{\partial^k \theta_n}{\partial x_1^k} + A f_k \frac{\partial^{k+1} \theta_n}{\partial x_1^{k+1}} \right) \\ & - \sum_{k=1}^{\infty} \left(Pe^{-2} f_k \frac{\partial^{k+2} \theta_n}{\partial x_1^{k+2}} + f_k \sum_{i=1}^{\infty} K_i \frac{\partial^{k+i} \theta_n}{\partial x_1^{k+i}} \right) = 0 \end{aligned} \quad (49)$$

It is observed that

$$\frac{\partial^{k+1} \theta_m}{\partial \tau \partial x_1^k} = \sum_{i=1}^{\infty} K_i(\tau) \frac{\partial^{i+k} \theta_m}{\partial x_1^{i+k}}$$

and so Eq. (49) becomes

$$\begin{aligned} & \left(\frac{\partial f_1}{\partial \tau} - \frac{1}{y} \frac{\partial}{\partial y} \frac{\partial f_1}{\partial y} \rightarrow A+K_1 \right) \frac{\partial \theta_m}{\partial x_1} \left[\frac{\partial f_2}{\partial \tau} - \frac{1}{y} \frac{\partial}{\partial y} \frac{\partial f_2}{\partial y} \rightarrow (A+K_1)f_1 + K_2 - Pe^{-2} \right] \frac{\partial^2 \theta_m}{\partial x_1^2} \\ & + \sum_{k=1}^{\infty} \left[\frac{\partial f_{k+2}}{\partial \tau} - \frac{1}{y} \frac{\partial}{\partial y} \frac{\partial f_{k+2}}{\partial y} \rightarrow (A+K_1)f_{k+1} + (K_2 - Pe^{-2})f_k + \sum_{i=3}^{k+2} K_i f_{k+2-i} \right] \frac{\partial^{k+2} \theta_m}{\partial x_1^{k+2}} \\ & = 0 \end{aligned} \quad (50)$$

with $f_0=1$

where

$$A = \frac{1}{V_0} \left(V_{m1} \left(\frac{1}{2} - y^2 \right) + V_{m2} \left(\frac{2}{\alpha+3} - y^{\alpha+1} \right) \right) \quad (51)$$

If equation (50) is satisfied by equating the coefficients of $\partial^k \theta_m / \partial x_1^k$ to zero, an infinite set of differential equations is generated

$$\frac{\partial f_1}{\partial \tau} = \frac{1}{y} \frac{\partial}{\partial y} \frac{\partial f_1}{\partial y} - (A+K_1) \quad (52)$$

$$\frac{\partial f_2}{\partial \tau} = \frac{1}{y} \frac{\partial}{\partial y} \frac{\partial f_2}{\partial y} - (A+K_1)f_1 + (Pe^{-2} - K_2) \quad (53)$$

$$\begin{aligned} \frac{\partial f_{k+2}}{\partial \tau} &= \frac{1}{y} \frac{\partial}{\partial y} \frac{\partial f_{k+2}}{\partial y} - (A+K_1)f_{k+1} + (Pe^{-2} - K_2)f_k - \sum_{i=3}^{k+2} K_i f_{k+2-i} \\ & \quad k = 1, 2, \dots \end{aligned} \quad (54)$$

Since θ_n will be chosen to satisfy the initial conditions on θ , at $\tau=0$, $\theta=\theta_n$ equation (45) implies that

$$f_k(0,y) = 0 \quad (k \neq 0) \quad (55)$$

Substituting (45) into (38d)

$$\frac{\partial}{\partial y} \left(\theta_n + \sum_{k=1}^{\infty} f_k(\tau,y) \frac{\partial^k \theta_n}{\partial x_1^k} \right) = 0 \quad \text{at } y = 0 \text{ \& } 1$$

$$\frac{\partial \theta_n}{\partial y} + \sum_{k=1}^{\infty} \frac{\partial f_k(\tau,y)}{\partial y} \frac{\partial^k \theta_n}{\partial x_1^k} = 0$$

$$\frac{\partial f_k}{\partial y}(\tau,0) = \frac{\partial f_k}{\partial y}(\tau,1) = 0 \quad (56)$$

and substituting (45) into (46)

$$\begin{aligned} \theta_n &= 2 \int_0^1 \left[y \left(\theta_n + \sum_{k=1}^{\infty} f_k(\tau,y) \frac{\partial^k \theta_n}{\partial x_1^k} \right) \right] dy \\ &= \theta_n + 2 \frac{\partial^k \theta_n}{\partial x_1^k} \int_0^1 y f_k dy \end{aligned}$$

which implies

$$\int_0^1 y f_k dy = 0 \quad (57)$$

By multiplying equation (52) by y and integrating with respect to y from 0 to 1

$$\frac{\partial}{\partial \tau} \int_0^1 y f_1 dy = \int_0^1 \frac{\partial}{\partial y} \left(\frac{\partial f_1}{\partial y} \right) dy - \int_0^1 \left(\frac{1}{v_0} [v_{m1} \left(\frac{1}{2} y - y^3 \right) + v_{m2} \left(\frac{2y}{\alpha+3} - y^{\alpha+2} \right)] + K_1 y \right) dy$$

and applying (56) and (57)

we obtain

$$K_1 = 0 \quad (58)$$

Applying the same procedure to equation (53)

$$\int_0^1 y \frac{\partial f_2}{\partial \tau} = \int_0^1 \frac{\partial}{\partial y} y \frac{\partial f_2}{\partial y} dy - \int_0^1 A f_1 y dy + \int_0^1 (Pe^{-2} - K_2) y dy$$

and using equation (57)

$$K_2(\tau) = Pe^{-2} + 2 \int_0^1 \left(\frac{v_{m1}}{v_0} y^3 + \frac{v_{m2}}{v_0} y^{\alpha+2} \right) f_1 dy \quad (59)$$

From (54) with $k=1$

$$\frac{\partial f_3}{\partial \tau} = \frac{1}{y} \frac{\partial}{\partial y} y \frac{\partial f_3}{\partial y} - A f_2 + (Pe^{-2} - K_2) f_1 - K_3 f_0$$

and noting that $f_0=1$

$$K_3 = 2 \int_0^1 \left[\frac{v_{m1}}{v_0} y^3 + \frac{v_{m2}}{v_0} y^{\alpha+1} \right] f_2 dy \quad (60)$$

In fact, Eq.(60) can be generalized as

$$K_{k+2}(\tau) = 2 \int_0^1 \left(\frac{v_{m1}}{v_0} y^3 + \frac{v_{m2}}{v_0} y^\alpha \right) f_{k+1} dy \quad (61)$$

In order to obtain the unsteady solution for $K_2(\tau)$ it is necessary to obtain the complete solution of equation (52)

for f_1 . This solution can be expressed in the form

$$f_1 = F_s(y) + F_t(\tau, y) \quad (62)$$

where $F_s(y)$ is the steady-state solution of equation (52), which independently satisfies the conditions given by equations (56) and (57). The time-dependent part of the solution of f_1 , $F_t(\tau, y)$, which must vanish as $\tau \rightarrow \infty$, satisfies a homogeneous differential equation with homogeneous boundary conditions and hence constitutes an eigenvalue problem which can readily be solved by the method of separation of variables.

Substituting Eq.(62) into Eq.(52) gives

$$\frac{d}{dy} y \frac{dF_s}{dy} = \frac{v_{m1}}{v_0} \left(\frac{y}{2} - y^3 \right) + \frac{v_{m2}}{v_0} \left(\frac{2y}{\alpha+3} - y^{\alpha+2} \right)$$

and integrating once

$$\frac{dF_s}{dy} = \frac{v_{m1}}{v_0} \left(\frac{y}{4} - \frac{y^3}{4} \right) + \frac{v_{m2}}{v_0} \left(\frac{y}{\alpha+3} - \frac{y^{\alpha+2}}{\alpha+3} \right) + \frac{C_1}{y}$$

where $C_1=0$ by virtue of the boundary conditions Eq.(56)

Further integration yields

$$F_s = \frac{v_{m1}}{v_0} \left(\frac{y^2}{8} - \frac{y^4}{16} \right) + \frac{v_{m2}}{v_0} \left[\frac{y^2}{2(\alpha+3)} - \frac{y^{\alpha+3}}{(\alpha+3)^2} \right] + C_2$$

and using Eq.(57)

$$\int_0^1 y F_s dy = 0$$

$$C_2 = -\frac{1}{24} \frac{V_{m1}}{V_0} - \frac{(\alpha+1)(\alpha+7)}{4(\alpha+3)^2(\alpha+5)} \frac{V_{m2}}{V_0} \quad (63)$$

Hence

$$F_s = \frac{V_{m1}}{V_0} \left[\frac{y^2}{8} - \frac{y^4}{16} - \frac{1}{24} \right] + \frac{V_{m2}}{V_0} \left[\frac{y^2}{2(\alpha+3)} - \frac{y^{\alpha+3}}{(\alpha+3)^2} - \frac{(\alpha+1)(\alpha+7)}{4(\alpha+3)^2(\alpha+5)} \right] \quad (64)$$

Now, $F_t(\tau, y)$ satisfies

$$\frac{\partial F_t}{\partial \tau} = \frac{1}{y} \frac{\partial}{\partial y} y \frac{\partial F_t}{\partial y}$$

By letting $F_t = T(\tau)U(y)$, we have

$$U \frac{dT}{d\tau} = \frac{T}{y} \frac{d}{dy} y \frac{dU}{dy} \quad (65)$$

and

$$\frac{1}{T} \frac{dT}{d\tau} = \frac{1}{U} \left[\frac{1}{y} \frac{dU}{dy} + \frac{d^2U}{dy^2} \right] = -\lambda^2 \quad (66)$$

The solutions of Eq.(66) are

$$T = S_1 \text{EXP}(-\lambda^2 \tau)$$

$$U = S_2 J_0(\lambda y) + S_3 Y_0(\lambda y)$$

and so

$$F_t = [S_1 J_0(\lambda y) + S_2 Y_0(\lambda y)] \text{EXP}(-\lambda^2 \tau) \quad (67)$$

Since at $y = 0$ $Y_0(0) \rightarrow \infty$, $S_2 = 0$. From Eq.(56)

$$\frac{\partial f_k}{\partial y}(\tau, 1) = 0$$

and since $\frac{dF_n}{dy}(1) = 0$, we have

$$J_1(\lambda) = 0 \quad (69)$$

Solution of Eq.(69) yields infinite number of eigenvalues and therefore the complete solution of F_t is

$$F_t = \sum_{n=1}^{\infty} A_n J_0(\lambda_n y) \text{EXP}(-\lambda_n^2 \tau) \quad (70)$$

where A_n is calculated using Eq.(55) $f_1(0, y) = 0$

$$\sum_{n=1}^{\infty} \int_0^1 y A_n J_0^2(\lambda_n y) \text{EXP}(-\lambda_n^2 \tau) dy$$

$$= \int_0^1 \left[\frac{v_{n1}}{v_0} \left(\frac{y^2}{8} \frac{y^4}{16} \frac{1}{24} \right) - \frac{v_{n2}}{v_0} \left[\frac{y^2}{2(\alpha+3)} \frac{y^{\alpha+3}}{(\alpha+3)^2} \frac{(\alpha+1)(\alpha+7)}{4(\alpha+3)^2(\alpha+5)} \right] \right] y J_0(\lambda_n y) dy$$

$$\therefore A_n \left(-\frac{J_0^2(\lambda_n)}{2} \right) = \int_0^1 \frac{v_{n1}}{v_0} \left(\frac{y^3}{8} \frac{y^5}{16} \frac{y}{24} \right) J_0(\lambda_n y) dy$$

$$+ \int_0^1 \frac{v_{n2}}{v_0} \left[\frac{y^3}{2(\alpha+3)} \frac{y^{\alpha+4}}{(\alpha+3)^2} \frac{(\alpha+1)(\alpha+7)y}{4(\alpha+3)^2(\alpha+5)} \right] J_0(\lambda_n y) dy$$

and by integrating by parts and the properties of Bessel functions,

$$\begin{aligned}
\int_0^1 y^3 J_0(\lambda_n y) dy &= \frac{1}{\lambda_n^4} [\lambda_n^3 J_1(\lambda_n) - \int_0^1 2(\lambda_n y)^2 J_1(\lambda_n y) d(\lambda_n y)] \\
&= \frac{1}{\lambda_n^4} [\lambda_n^3 J_1(\lambda_n) - 2\lambda_n^2 J_2(\lambda_n)] \\
&= -2 \frac{J_2(\lambda_n)}{\lambda_n^2}
\end{aligned}$$

$$\frac{1}{16} \int_0^1 y^5 J_0(\lambda_n y) dy = -\frac{J_2(\lambda_n)}{4\lambda_n^2} + \frac{J_3(\lambda_n)}{2\lambda_n^3}$$

$$\int_0^1 y J_0(\lambda_n y) dy = J_1(\lambda_n) = 0$$

Therefore,

$$\begin{aligned}
A_n \left[-\frac{J_0^2(\lambda_n)}{2} \right] &= -\frac{V_{n1}}{V_0} \left[-\frac{J_2(\lambda_n)}{4\lambda_n^2} \frac{J_2(\lambda_n)}{4\lambda_n^2} \frac{J_3(\lambda_n)}{2\lambda_n^3} \right] \\
&\quad - \frac{V_{n2}}{V_0} \left[\frac{J_2(\lambda_n)}{(\alpha+3)\lambda_n^2} \frac{1}{(\alpha+3)^2} \int_0^1 y^{\alpha+1} J_0(\lambda_n y) dy \right]
\end{aligned}$$

and the complete solution for f_1 is then given by

$$\begin{aligned}
f_1 &= \frac{V_{n1}}{V_0} \left(\frac{y^2}{8} - \frac{y^4}{16} - \frac{1}{24} \right) + \frac{V_{n2}}{V_0} \left[\frac{y^2}{2(\alpha+3)} - \frac{y^{\alpha+1}}{(\alpha+3)^2} - \frac{(\alpha+1)(\alpha+7)}{4(\alpha+3)^2(\alpha+5)} \right] \\
&\quad + \sum_{n=1}^{\infty} A_n J_0(\lambda_n y) \exp(-\lambda_n \tau) \tag{71}
\end{aligned}$$

where A_n 's are given by

$$A_n = \frac{V_{n1}}{V_0 \lambda_n^3 J_0^2(\lambda_n)} + \frac{V_{n2}}{V_0} \frac{1}{\lambda_n J_0^2(\lambda_n)} \left[\frac{J_2(\lambda_n)}{(\alpha+3)\lambda_n^2} + \frac{1}{(\alpha+3)^2} \int_0^1 y^{\alpha+4} J_0(\lambda_n y) dy \right] \tag{72}$$

and the eigenvalues λ_n 's must satisfy

$$J_1(\lambda_n) = 0 \quad (73)$$

Equation (71) can now be substituted into equation (59) to yield the general solution for $K_2(\tau)$

$$K_2(\tau) = Pe^{-2} + \frac{1}{192} \frac{V_{n1}^2}{V_0^2} + \frac{(\alpha+1)(\alpha+11)}{12(\alpha+3)(\alpha+5)(\alpha+7)} \frac{V_{n1}V_{n2}}{V_0^2} + \frac{(\alpha+1)^2}{2(\alpha+5)(\alpha+3)^3} \frac{V_{n2}^2}{V_0^2} - 4 \sum_{n=1}^{\infty} (B_{n1} + B_{n2}) \text{EXP}(-\lambda_n^2 \tau) \quad (74)$$

where

$$B_{n1} = -\frac{1}{2} \frac{V_{n1}}{V_0} \frac{J_2(\lambda_n)}{\lambda_n^2} A_n \quad (75a)$$

$$B_{n2} = -\frac{1}{2} \frac{V_{n2}}{V_0} A_n \int_0^1 y^{\alpha+2} J_0(\lambda_n y) dy \quad (75b)$$

The nomenclature used here conforms to that used by Gill and Sankarasubramanian (1970). Hence the results presented here for f_1 , A_n , $K_2(\tau)$, B_n , etc. were checked to reduce to those of Gill and Sankarasubramanian for Newtonian fluids when α is set equal to 1. On the other hand, the time-independent dispersion coefficient for Ellis model fluids given by the limit of equation (74) as $\tau \rightarrow \infty$, agrees with that of Fan and Hwang (1965).

The higher order coefficients in the generalized dispersion model can be determined by a solution of equation (61) for the appropriate value of k . This necessitates

solving equation (53) or (54) to order $k-1$ which is a straightforward but algebraically tedious task. Gill and Sankarasubramanian (1970) have shown that for Newtonian fluid $K_3(\tau \rightarrow \infty) = -4.34 \cdot 10^{-5}$ and the higher order coefficients will decrease in magnitude further. As for Ellis model, equation (53) has been solved for the steady state solution for f_2 in order to obtain the solution for $K_3(\omega)$. A few values of K_3 were obtained for different polymers under the condition of $\tau_R/\tau_K=2.5$. $K_3(\omega)$ is $4.608 \cdot 10^{-5}$ for $\alpha=3.59$ whereas the corresponding $K_2(\omega)$ is $4.421 \cdot 10^{-3}$. For $\alpha=2.50$ $K_3(\omega)$ is $5.482 \cdot 10^{-5}$ and K_2 is $4.986 \cdot 10^{-3}$. Therefore we see that $K_2(\omega)$ is more than two orders of magnitude greater than $K_3(\omega)$ for Ellis model fluids. Booras and Krantz (1976) also have proven that for power law fluid for all values of n , $K_3(\omega)$ is significantly smaller than $K_2(\omega)$. Thus it appears reasonable to assume that $K_3(\omega) \ll K_2(\omega)$ for all values of τ ; hence the generalized dispersion model can be approximated by only one term in equation (48)

i.e.

$$\frac{\partial \theta_m}{\partial \tau} = K_2 \frac{\partial^2 \theta_m}{\partial X_1^2} \quad (76)$$

The solution of equation (76) with conditions

$$\begin{aligned} \theta(0, X_1, y) &= 1 & |X_1| &\leq X_s \\ \theta(0, X_1, y) &= 0 & |X_1| &> X_s \\ \theta(\tau, \infty, y) &= 0 \end{aligned}$$

$$\frac{\partial \theta}{\partial y}(\tau, X_1, 0) = \frac{\partial \theta}{\partial y}(\tau, X_1, 1) = 0$$

is obtained by the method of separation of variables.

Let $\theta_n = Z(X_1)T(\tau)$, so that

$$Z \frac{dT}{d\tau} = K_2(\tau) T \frac{d^2 Z}{dX_1^2} \quad (77)$$

and introducing the separation constant β^2

$$\frac{1}{K_2 T} \frac{dT}{d\tau} = -\frac{1}{Z} \frac{d^2 Z}{dX_1^2} = -\beta^2 \quad (78)$$

The problem becomes

$$Z''(X_1) + \beta^2 Z = 0 \quad (79a)$$

$$\frac{dT}{T} = -\beta^2 K_2(\tau) d\tau \quad (79b)$$

the solutions of which are

$$Z = c_1 \cos(\beta X_1) + c_2 \sin(\beta X_1)$$

$$T = c_3 \exp(-\beta^2 \zeta)$$

where

$$\zeta = \int_0^\tau K_2(\eta) d\eta$$

c_1 , c_2 , and c_3 are constants

Hence, θ_n may be written in terms of Fourier integral

$$\theta_n = \int_0^\infty [A_\beta \cos(\beta X_1) + B_\beta \sin(\beta X_1)] \exp(-\beta^2 \zeta) d\beta \quad (80)$$

Then

$$\Theta_n(0, X_1) = \int_0^{\infty} [A_\beta \cos(\beta X_1) + B_\beta \sin(\beta X_1)] d\beta \quad (82)$$

and using Fourier transformation, $\Theta_n(0, X_1)$ may be expressed as

$$\Theta_n(0, X_1) = \frac{1}{\pi} \int_0^{\infty} \int_{-\infty}^{\infty} \Theta_n(0, s) \cos[\beta(s - X_1)] ds d\beta \quad (-\infty < X_1 < \infty) \quad (83)$$

Comparing Eq. (82) and (83)

$$A_\beta \cos(\beta X_1) + B_\beta \sin(\beta X_1) = \frac{1}{\pi} \int_{-\infty}^{\infty} \Theta_n(0, s) \cos[\beta(s - X_1)] ds$$

which implies

$$\begin{aligned} \Theta_n &= \frac{1}{\pi} \int_0^{\infty} \left(\int_{-\infty}^{\infty} \Theta_n(0, s) \cos[\beta(s - X)] ds \right) \exp(-\beta^2 \zeta) d\beta \\ &= \frac{1}{\pi} \int_{-\infty}^{\infty} \Theta_n(0, s) \left(\int_0^{\infty} \cos[\beta(s - X_1)] \exp(-\beta^2 \zeta) d\beta \right) ds \end{aligned} \quad (84)$$

Letting

$$v^2 = \beta^2 \zeta \quad (84a)$$

$$g = \frac{s - X_1}{2\sqrt{\zeta}} \quad (84b)$$

we have

$$\int_0^{\infty} \cos[\beta(s - X_1)] \exp(-\beta^2 \zeta) d\beta = \frac{1}{2} \sqrt{\frac{\pi}{\zeta}} \exp\left[-\frac{(s - X_1)^2}{4\zeta}\right]$$

and therefore

$$\begin{aligned}
 \Theta_n &= \frac{1}{\pi} \int_{-\infty}^{\infty} \Theta_n(0, s) \frac{1}{2} \sqrt{\frac{\pi}{\zeta}} \text{EXP} \left[-\frac{(s-X_1)^2}{4\zeta} \right] ds \\
 &= \frac{1}{2\sqrt{\pi\zeta}} \int_{-\infty}^{\infty} \Theta_n(0, s) \text{EXP} \left[-\frac{(s-X_1)^2}{4\zeta} \right] ds \\
 &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \Theta_n(0, X_1 + 2g\sqrt{\zeta}) \text{EXP}(-g^2) dg
 \end{aligned} \tag{85}$$

Then, using the conditions :

$$\begin{aligned}
 \Theta &= \Theta_n = \Theta_n(0, X_1) = 1 & |X_1| \leq \%X_s \\
 \Theta &= \Theta_n = \Theta_n(0, X_1) = 0 & |X_1| > \%X_s
 \end{aligned}$$

we finally obtain

$$\begin{aligned}
 \Theta_n &= \frac{1}{2\sqrt{\pi\zeta}} \int_{-\%X_s}^{\%X_s} \text{EXP} \left[-\frac{(s-X_1)^2}{4\zeta} \right] ds \\
 &= \frac{1}{\sqrt{\pi}} \int_{-(\%X_s+X_1)/2\sqrt{\zeta}}^{(\%X_s-X_1)/2\sqrt{\zeta}} \text{EXP}(-g^2) dg \\
 &= \frac{1}{2} \left[\text{erf} \left(\frac{\%X_s+X_1}{2\sqrt{\zeta}} \right) + \text{erf} \left(\frac{\%X_s-X_1}{2\sqrt{\zeta}} \right) \right]
 \end{aligned} \tag{86}$$

where

$$\zeta = \int_0^{\tau} K_2(\eta) d\eta \tag{87}$$

$$\begin{aligned}
&= [Pe^{-2} + \frac{1}{192} \frac{v_{m1}^2}{v_0^2} + \frac{(\alpha+1)(\alpha+11)}{12(\alpha+3)(\alpha+5)(\alpha+7)} \frac{v_{m1}v_{m2}}{v_0^2} \\
&+ \frac{(\alpha+1)^2}{2(\alpha+5)(\alpha+3)^3} \frac{v_{m1}^2}{v_0^2}] \tau - 4 \sum_{m=1}^{\infty} \frac{1}{\lambda_m^2} (B_{m1} + B_{m2}) [1 - \exp(-\lambda_m^2 \tau)]
\end{aligned}$$

In order to analyze the dispersion behavior of Ellis model fluids, a new dimensionless variable P is defined as

$$P = \frac{\tau_R}{\tau_k} \quad (88)$$

then we have the following

$$\frac{v_{m1}}{v_0} = \frac{1}{1+H} \quad (89a)$$

$$\frac{v_{m2}}{v_0} = \frac{H}{1+H} \quad (89b)$$

where

$$H = \frac{v_{m2}}{v_{m1}} = \frac{2}{\alpha+1} P^{\alpha-1} \quad (89c)$$

III. RESULTS AND DISCUSSIONS

Some commercial polymers are used in this study. Their properties for these three models are listed in Table 1.

A. Comparison of KD/R^4 values by Taylor-Aris dispersion theory for different models

From equations (29), (31) and (34), the KD/R^4 values are calculated for different wall shear stress τ_R . Figures 1 and 2 show the plots of KD/R^4 under different τ_R for two commercial polymers: Ethylene ethyl acrylate at 463k and Polystyrene at 483k.

From these figures we can see that at high shear stress ($>10^5$) the KD/R^4 values of these three models are almost non-distinguishable, but as τ_R decreases, the deviation among them becomes significant. We can see a tremendous difference between the three-parameter models, i.e. Carreau model and Ellis model, and the two-parameter power-law model. For example, for PS with $\tau_R = 5 \times 10^4$, the results of Carreau model and Ellis model are comparable while the results of power-law model are one order of magnitude less than those of the two three-parameter models. As τ_R decreases below 1×10^4 , the difference between the three-parameter and power-law models is more pronounced (>four orders of magnitude).

This result is expected. Since at low shear stress near the axis or at low pressure gradient, the fluid is within the

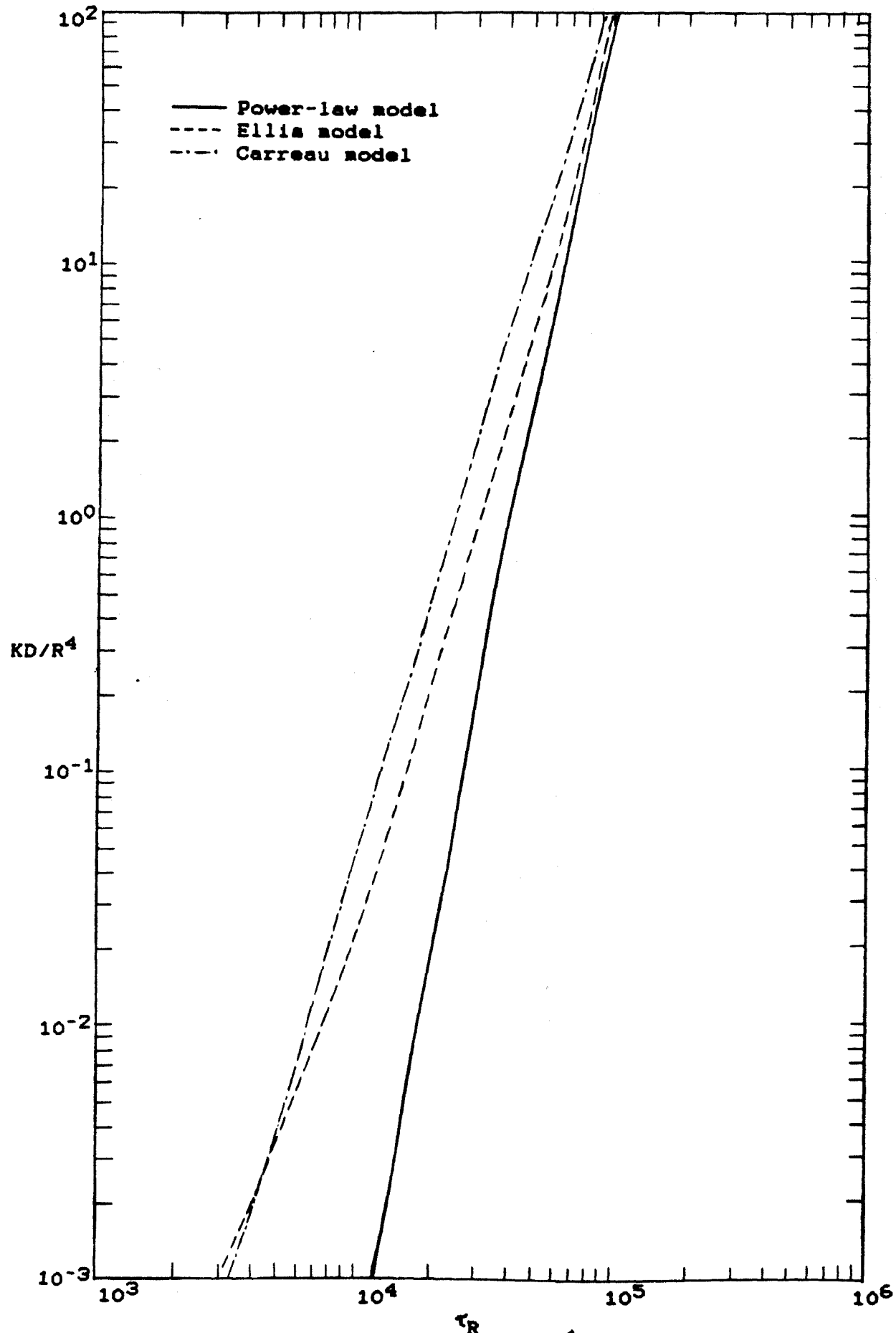


Fig. 1. Dispersion property τ_R KD/R^4 of ethylene ethyl acrylate, DPDA-6169 at 483k vs. shear stress at tube wall for three different models

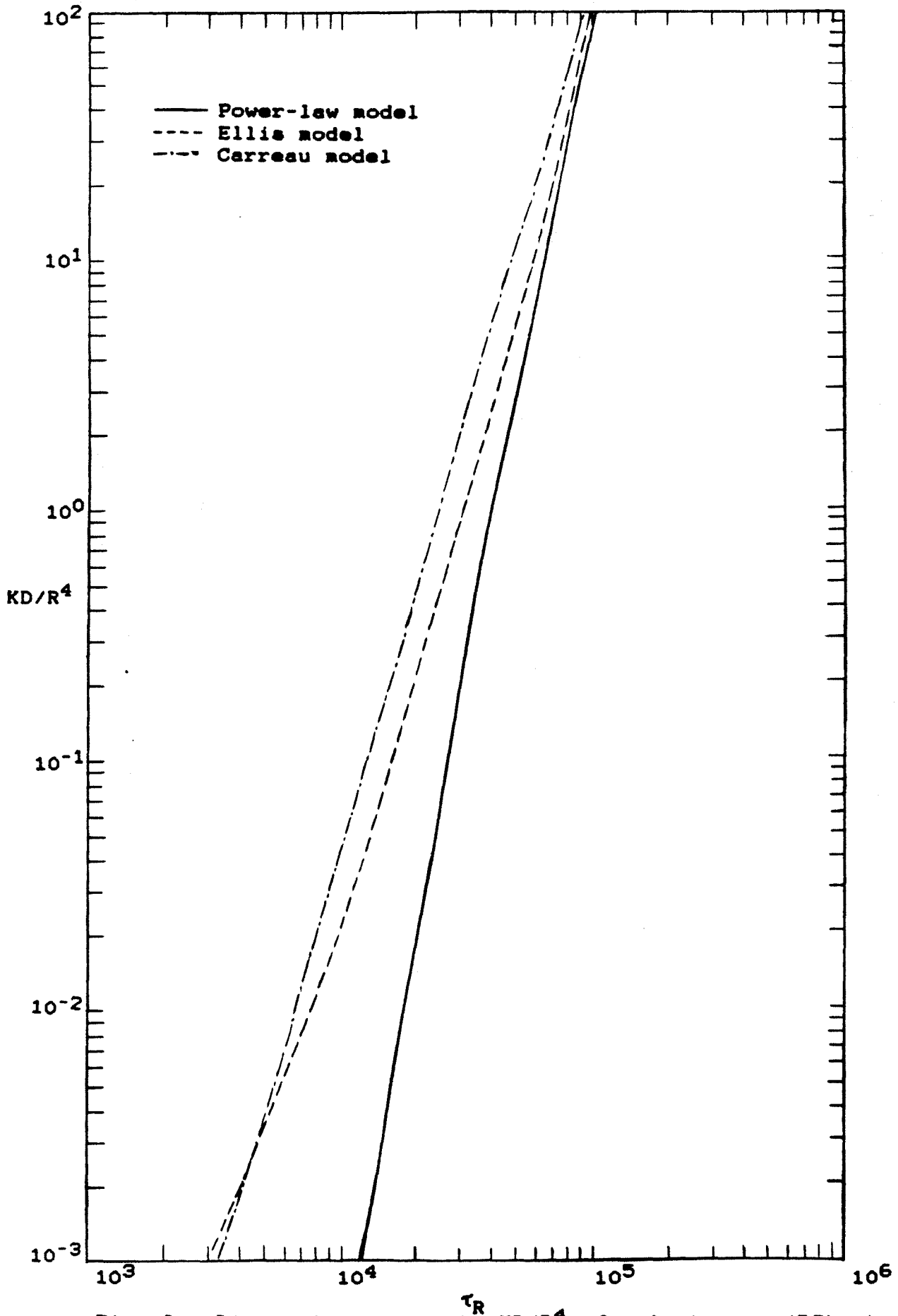


Fig. 2. Dispersion property KD/R^4 of polyatylene (PS) at 483K vs. wall shear stress for three different models

low Newtonian regime, where power law can not be used to predict the behavior correctly. On the other hand we know that the three-parameter Carreau model and Ellis model include the low Newtonian region and power law region. For tube flow the shear stress increases linearly from zero on the axis to τ_R at the wall. Thus, the fluid exhibits Newtonian behaviour near the axis (plug flow) for any pressure gradient. Thus, straightly speaking, power-law model is not applicable to pipe flow. There is no doubt that the calculated KD/R^4 values from these two models are of the same magnitude even at low shear stress, and power law applied to this low shear stress region becomes more unreliable since its value is very far from those obtained from these two three-parameter models.

Thus we know that from the results of the Taylor-Aris dispersion theory it is more appropriate to use three-parameter model than power-law model. From this point of view we would like to see what will happen if we apply the three-parameter Ellis model to the generalized dispersion theory of Gill and Sankarasubramanian. It may have some very interesting implications which were not shown in the Newtonian fluids and power-law fluids. In next section, the three-parameter Ellis model is applied to the generalized dispersion theory of Gill and Sankarasubramanian and the results will be compared with those obtained by Booras and Krantz (1976) who used the power-law model.

B. Results of the generalized dispersion theory of Ellis fluid in pipe flow

Figures 3,4 and 5 give the plots of K_2-Pe^{-2} as a function of τ under different driving force P for three commercial polymers. For comparison, K_2-Pe^{-2} for power-law fluid is also shown in each figure. In determining K_2 from Eq. (74), the infinite series was truncated such that the leading term discarded resulted in less than a 0.1% change in the value of K_2 .

Furthermore, the time-dependent behavior of the dispersion coefficient $k_2(\tau)$ for all Ellis model fluids is similar in that these fluids approach their steady state value at approximately the same rate.

It is seen from these figures that the dispersion coefficient varies rapidly with τ in the region of $\tau \leq 0.1$, and then it changes more slowly until K_2 becomes constant at $\tau \geq 0.3$. As P increases, the dispersion coefficient of the Ellis model approaches that of the power-law model, while as P decreases, $K_2(\infty)-Pe^{-2}$ approaches the value of Newtonian fluid which equals $5.2083 \cdot 10^{-3}$.

It may make clearer to know the relation between radial distance ξ and shear rate τ under different driving force P ($=\tau_R/\tau_k$). Differentiating equation (19) with respect to ξ , we have the relation as

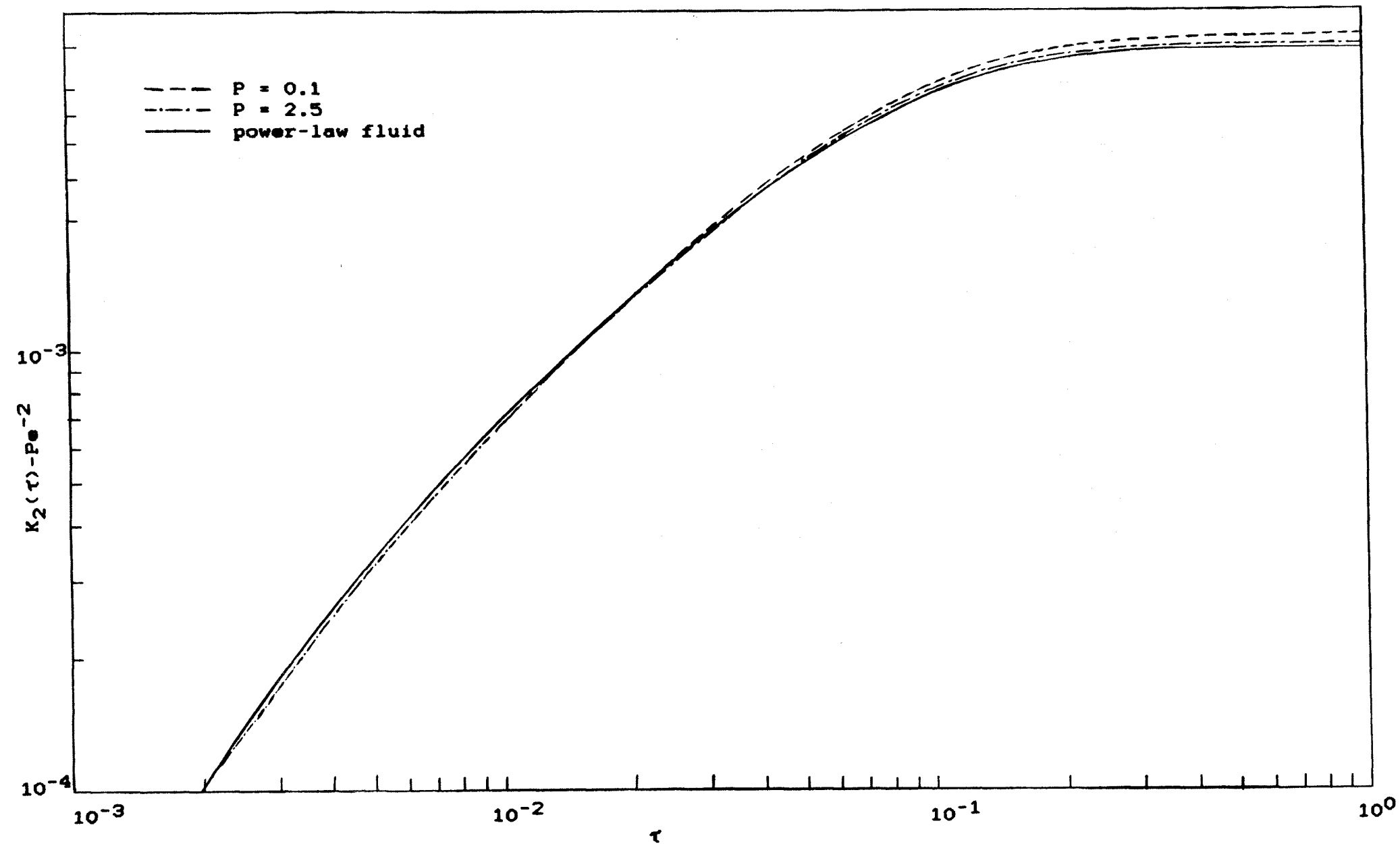


Fig. 3. Comparison of $K_2(\tau) - Pe^{-2}$ of Polypropylene (PP) at 463K as a function of dimensionless time for Ellis model with the result of power-law model

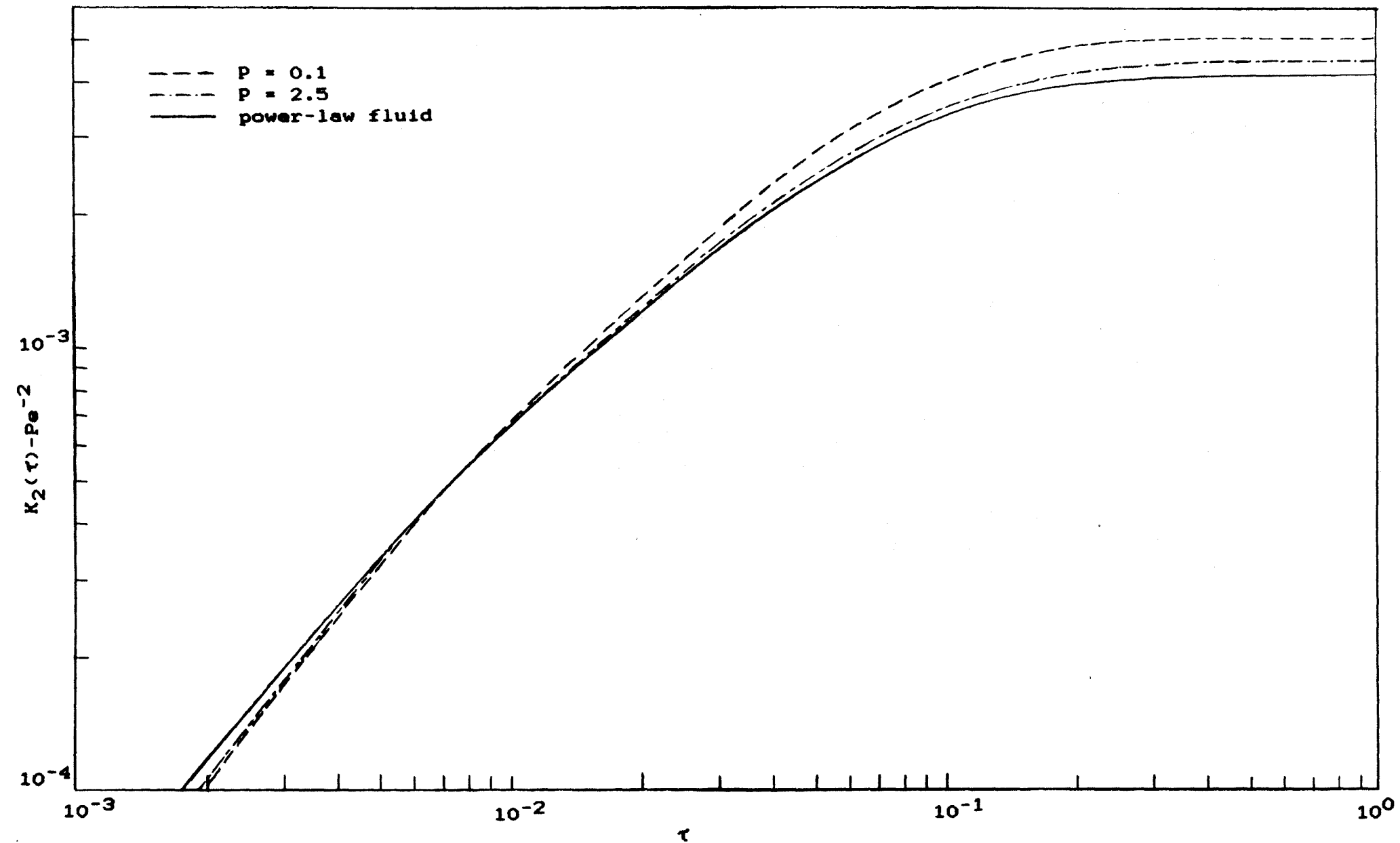


Fig. 4. Comparison of $K_2(\tau) - Pe^{-2}$ of styrene acrylonitrile at 493K as a function of dimensionless time for Ellis model with the result of power-law model

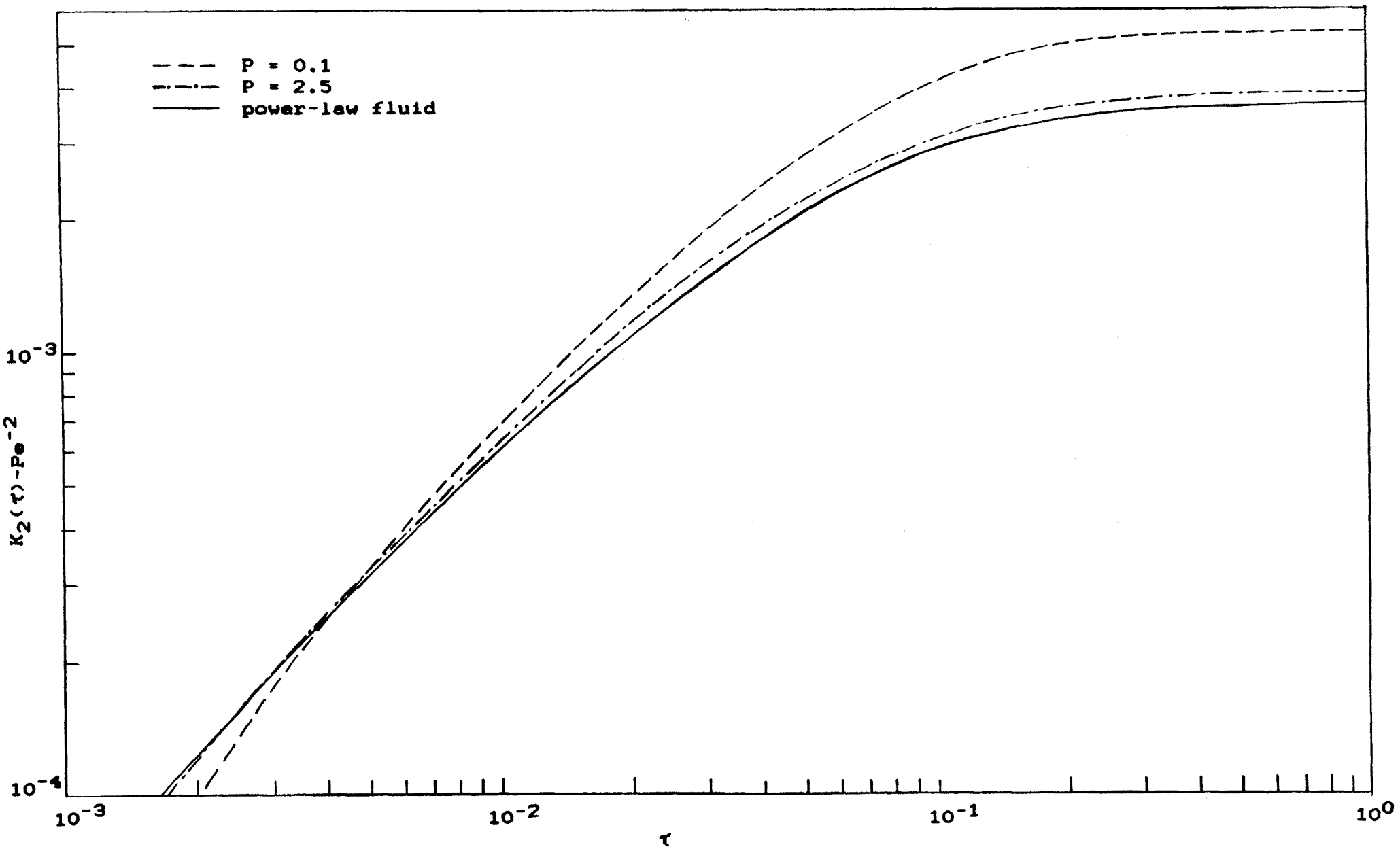


Fig. 5. Comparison of $K_2(\tau) - Pe^{-2}$ of High Impact Polystyrene (HIPS) at 463k as a function of dimensionless time for Ellis model with the result of power-law model

$$\tau = \frac{\tau_x}{\tau_0} P\xi [1 + (P\xi)^{\alpha-1}]$$

Figure 6 gives a plot of shear rate τ against dimensionless radial distance ξ for $\alpha=3.59$. It is seen that the shear rate difference between $P=0.1$ and $P=1.0$ is significant. At $\xi=0.4$ the shear rate for $P=1.0$ is more than ten times that for $P=0.1$. As ξ increases, the ratio is even more. So it is reasonable that we treat the Ellis model fluid under low P as near lower Newtonian regime and within power law region or higher Newtonian regime at large P .

The results of Figures 3,4 and 5 are, therefore, expected. As P increases, the dispersion coefficient approaches the value of power-law fluid, and at low P the dispersion coefficient is near the value of Newtonian fluid.

Figure 7 shows a plot of $K_2(\omega) - Pe^{-2}$ vs. α . It indicates that under $P=1.5$, $K_2(\omega) - Pe^{-2}$ exhibits a maximum value of $5.241 \cdot 10^{-3}$ at $\alpha=1.23$; under $P=3.5$ the maximum value of $K_2(\omega) - Pe^{-2}$ is $5.247 \cdot 10^{-3}$ at $\alpha=1.48$. Booras and Krantz reported similar observation for power law fluid; the maximum value is reached at $n=0.729$ with $K_2 - Pe^{-2} = 5.28 \cdot 10^{-3}$. For Ellis model, the maximum value depends on P . Erdogan (1967) commented that it was rather remarkable that pseudoplastic fluids ($\alpha > 1$) could cause more dispersion than Newtonian fluids. Indeed, one might expect $K_2(\omega)$ to decrease as α increases due to the decreased axial dispersion associated with progressively more blunt velocity profile.

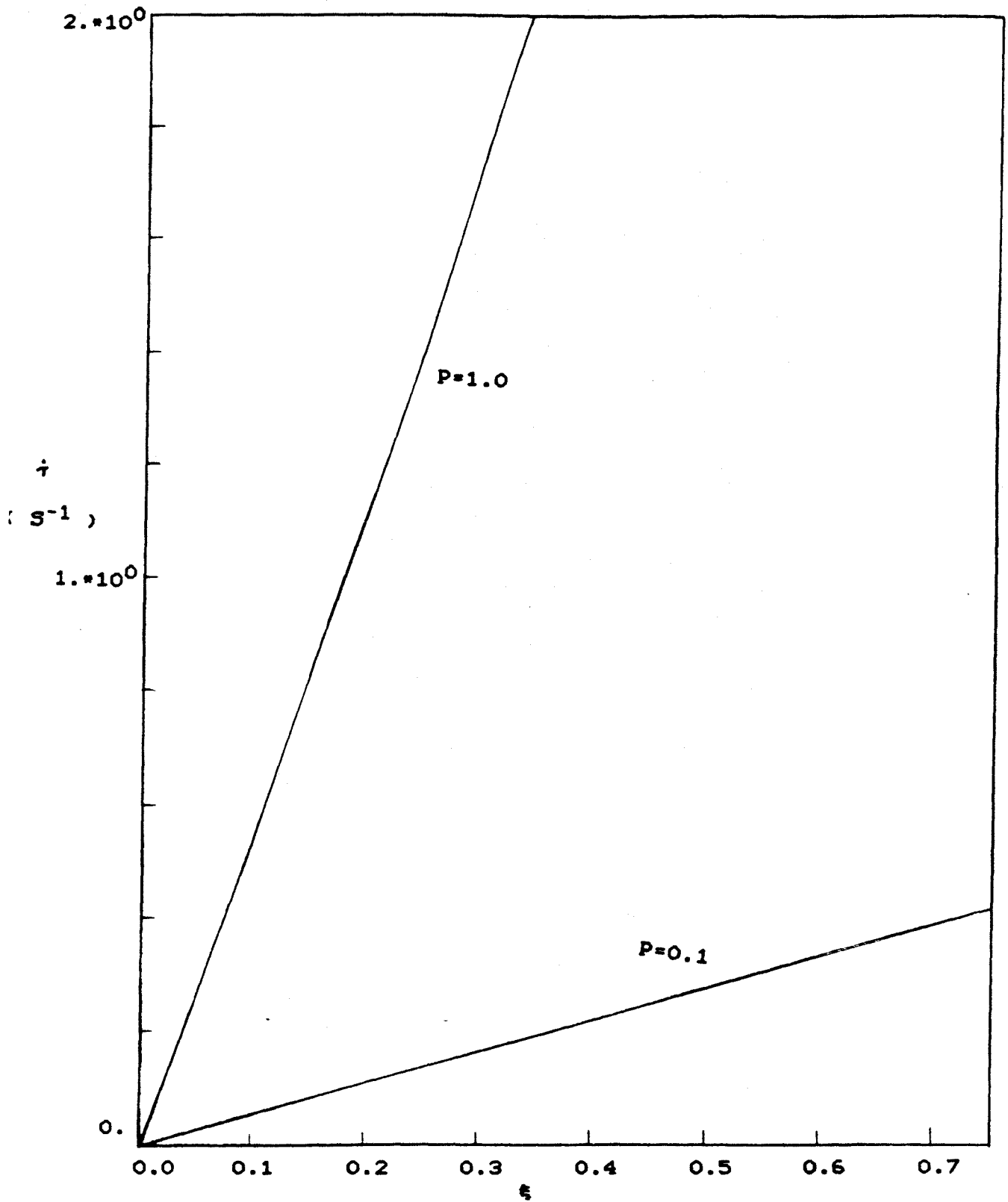


Fig. 6. Shear rate as a function of dimensionless distance for $P=0.1$ and $P=1.0$

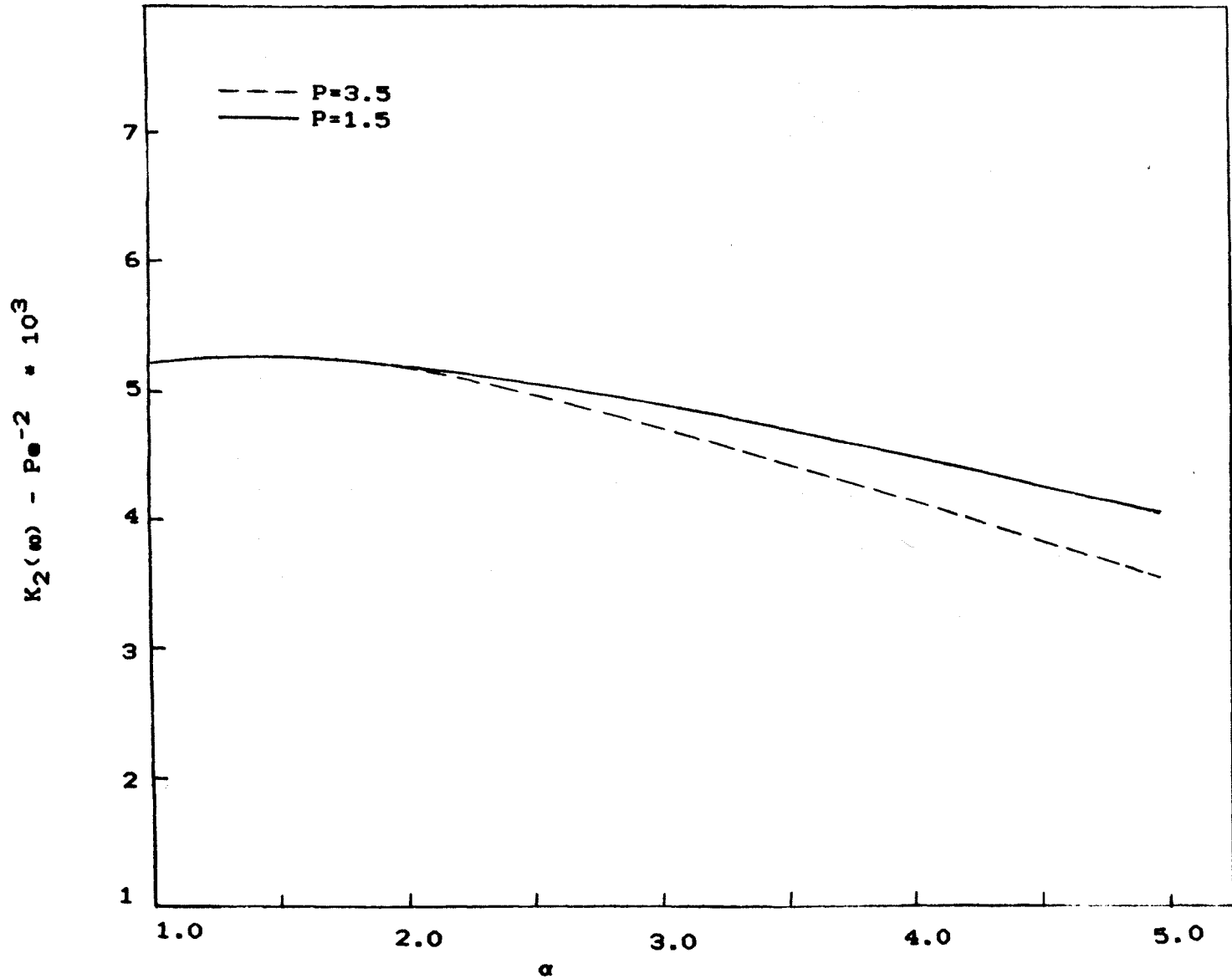


Fig. 7. Dispersion coefficient based on maximum velocity V_0 under different P as a function of flow behaviour index for Ellis model fluids

The unexpected behavior that $K_2(\infty)$ attains a maximum is a consequence of the choice of the velocity scale V_0 . Let us define another dispersion coefficient K_2^* , nondimensionalized with the average velocity V_x rather than the maximum velocity, whose relationship to K_2 is given by

$$K_2^* - Pe^{-2} = \left(\frac{V_0}{V_x} \right)^2 (K_2 - Pe^{-2}) = \left(\frac{1+H}{\frac{1}{2} + \frac{\alpha+1}{\alpha+3}H} \right)^2 (K_2 - Pe^{-2}) \quad (90)$$

This modified dispersion coefficient K_2^* is plotted against α in Figure 8. It is seen that there is no maximum and K_2^* decreases monotonically with α . The monotonic decreasing of K_2^* with α is consistent with non-Newtonian behavior, because larger α implies stronger shear-thinning behavior at a given pressure gradient and hence more convective transport giving a smaller dispersion. The behavior of K_2 is a consequence of the ratio V_0/V_x which increases with increasing α thus counterbalancing the decrease of K_2^* with increasing α .

There are two reasons that the definition of K_2 is preferable to that of K_2^* . First, the former definition was used by Gill and co-workers, Fan and co-workers, Erdogan, and Booras and Krantz, and permits direct comparison with their results. Second, the more significance is the fact that K_2 is far less sensitive to α than K_2^* . From Figure 7 that the $K_2(\infty) - Pe^{-2}$ varies only a few percents over the range of flow behavior indices $1 \leq \alpha \leq 2$, this includes a broad range of

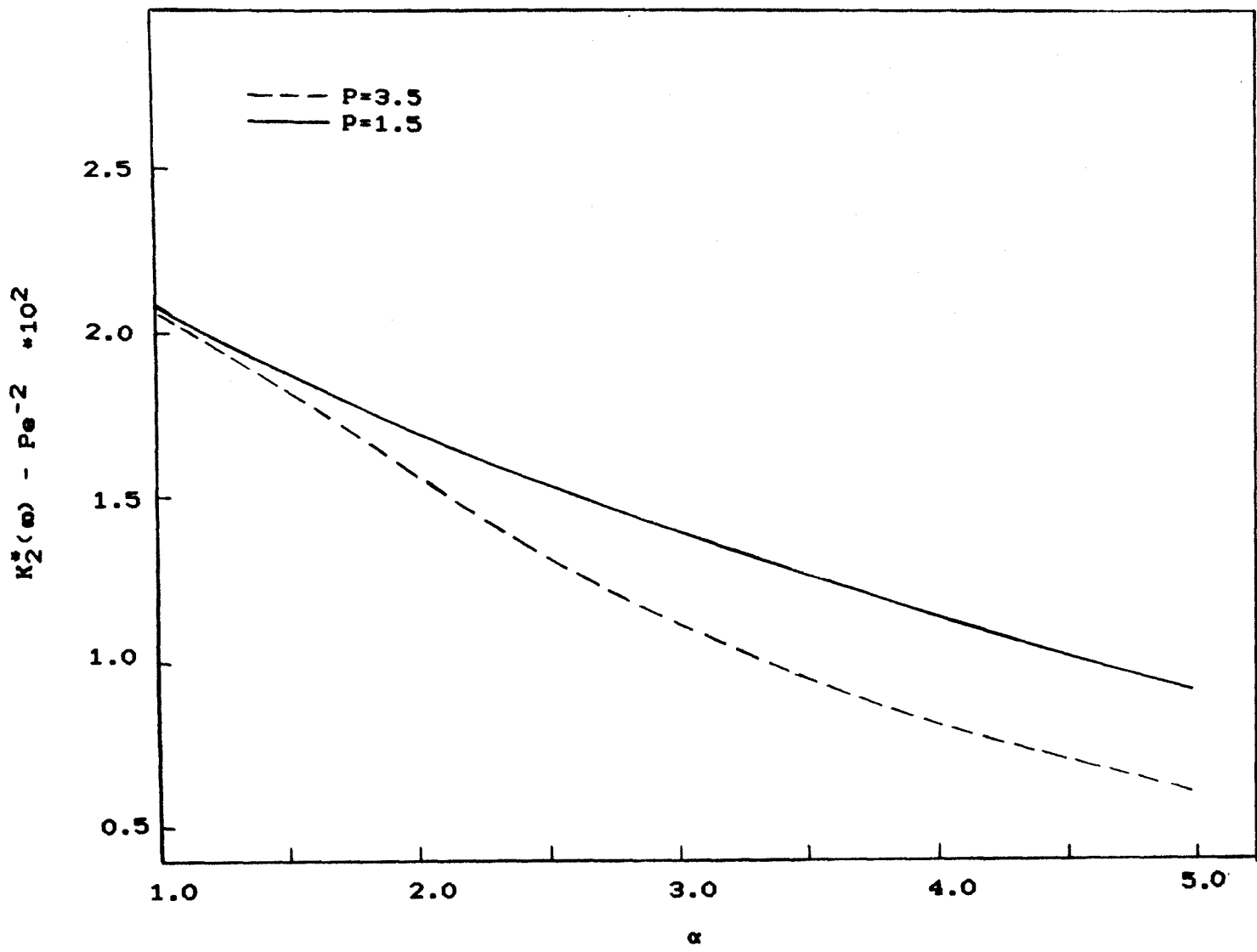


Fig. 8. Dispersion coefficient based on mean velocity under different P as a function of flow behaviour index for Ellis model fluids

pseudoplastic and Newtonian behaviors, and the Newtonian value of the dispersion coefficient $K_2(\infty)$ can be used with little error. On the other hand if we use K_2^* as a definition, it is seen from Fig 8 that $K_2^*(\infty)$ decreases as α increases. The Newtonian value of the dispersion coefficient $K_2^*(\infty)$ can not be used to predict the pseudoplastic behavior even though α value is near 1, since it would cause large error.

We would like to see how significant the Peclet number will effect the dispersion coefficient. As mentioned before at low shear stress dispersion coefficient approaches that of Newtonian fluid. Substituting equations (20a), (20b) and (88) into the definition of the Peclet number, we have

$$Pe = \frac{RV_0}{D} \frac{R}{D} = \frac{R^2}{D^2} (V_{m1} + V_{m2}) \quad (91)$$

$$= \frac{R^2}{D} \frac{\tau_x}{\tau_0} \left(\frac{P}{2} + \frac{P^\alpha}{\alpha+1} \right) \quad (92)$$

We assume a typical liquid phase diffusivity, as mentioned in the INTRODUCTION, $D=10^{-5}$ cm²/s, and tube radius $R=0.1$ cm for three different sets of (α, τ_x, τ_0) under the same condition $P=0.1$. The results are shown in Figures 9,10 and 11. It is seen that at lower τ_x/τ_0 the effect of Peclet number is more noticeable when Figure 11 is compared with Figure 9.

A plot of θ_n vs. X is shown in Figure 12 and Figure 13 for $\alpha=4.8$ and $\alpha=3.59$ respectively at $X_n=0.019, Pe=1000$ and

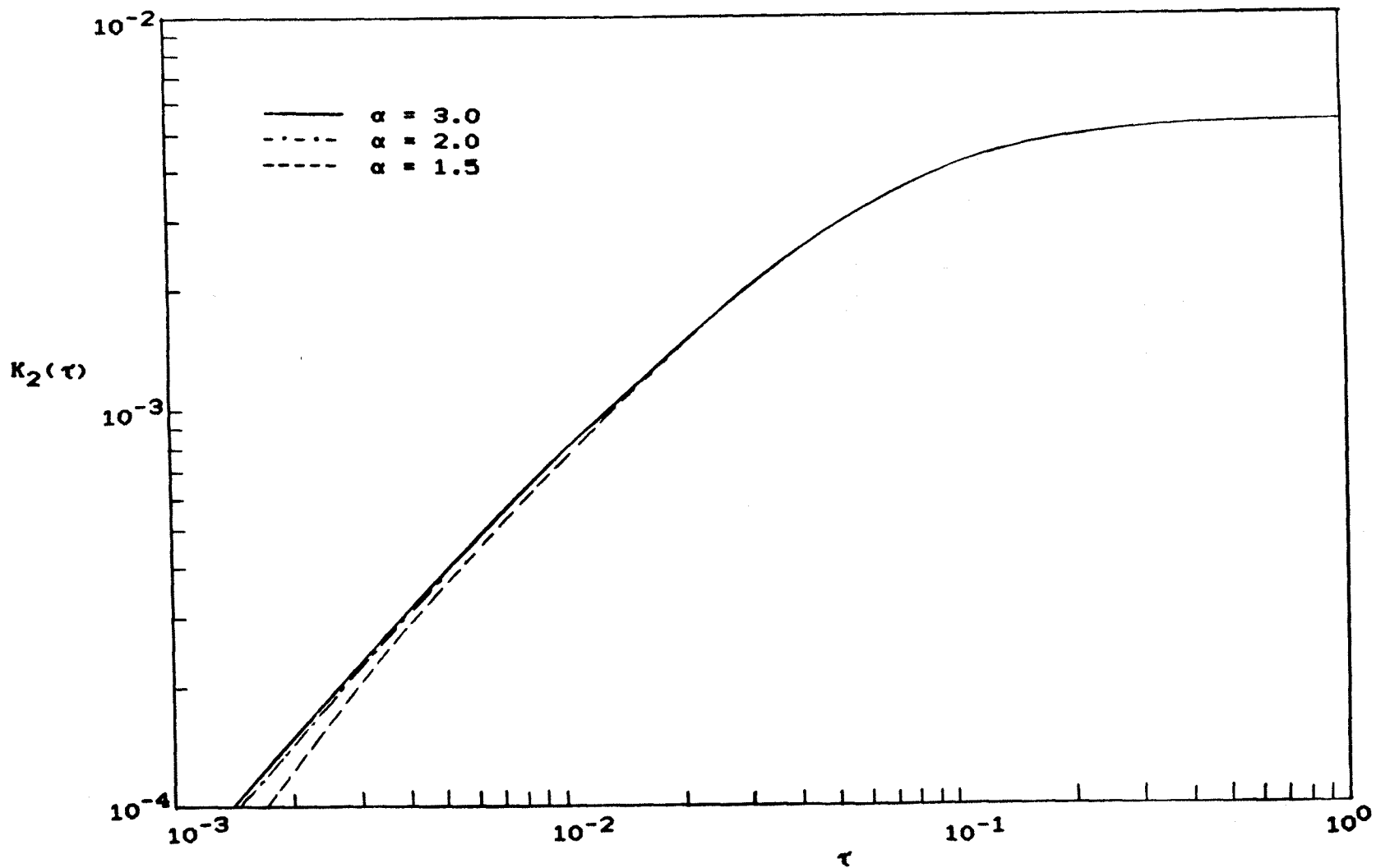


Fig. 9. Plot of $K_2(\tau)$ against dimensionless time τ under $P=0.1$ for three different set of polymer having the same τ_0 ($=3.2 \times 10^3$ NS/m²) and $\tau_{1/2}$ ($=9.06 \times 10^3$ N/m²)

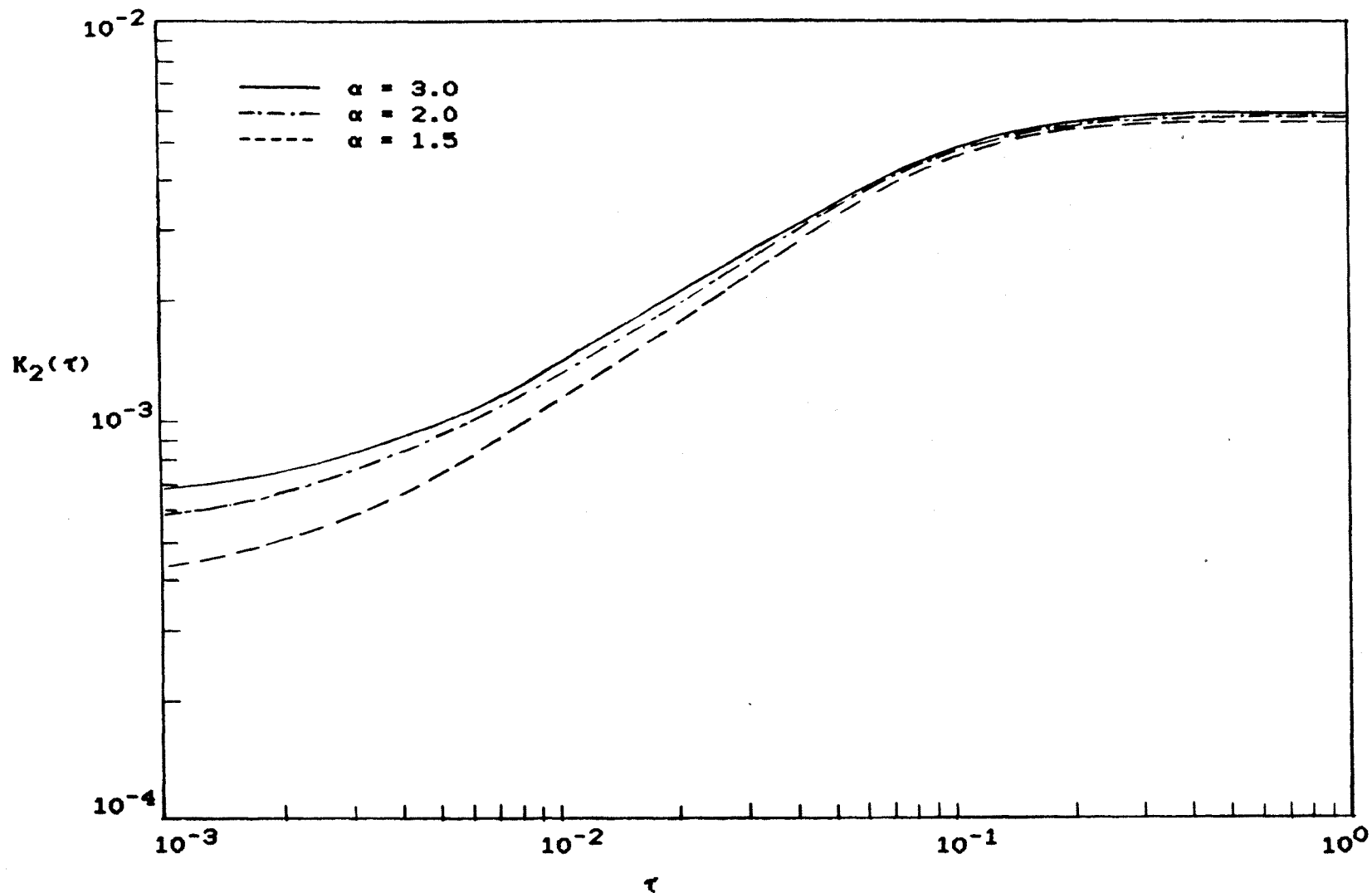


Fig. 10. Plot of $K_2(\tau)$ against dimensionless time τ under $P=0.1$ for three different set of polymers having the same τ_0 ($=2.15 \cdot 10^4$ NS/m²) and $\tau_{1/2}$ ($=1.68 \cdot 10^4$ N/m²)

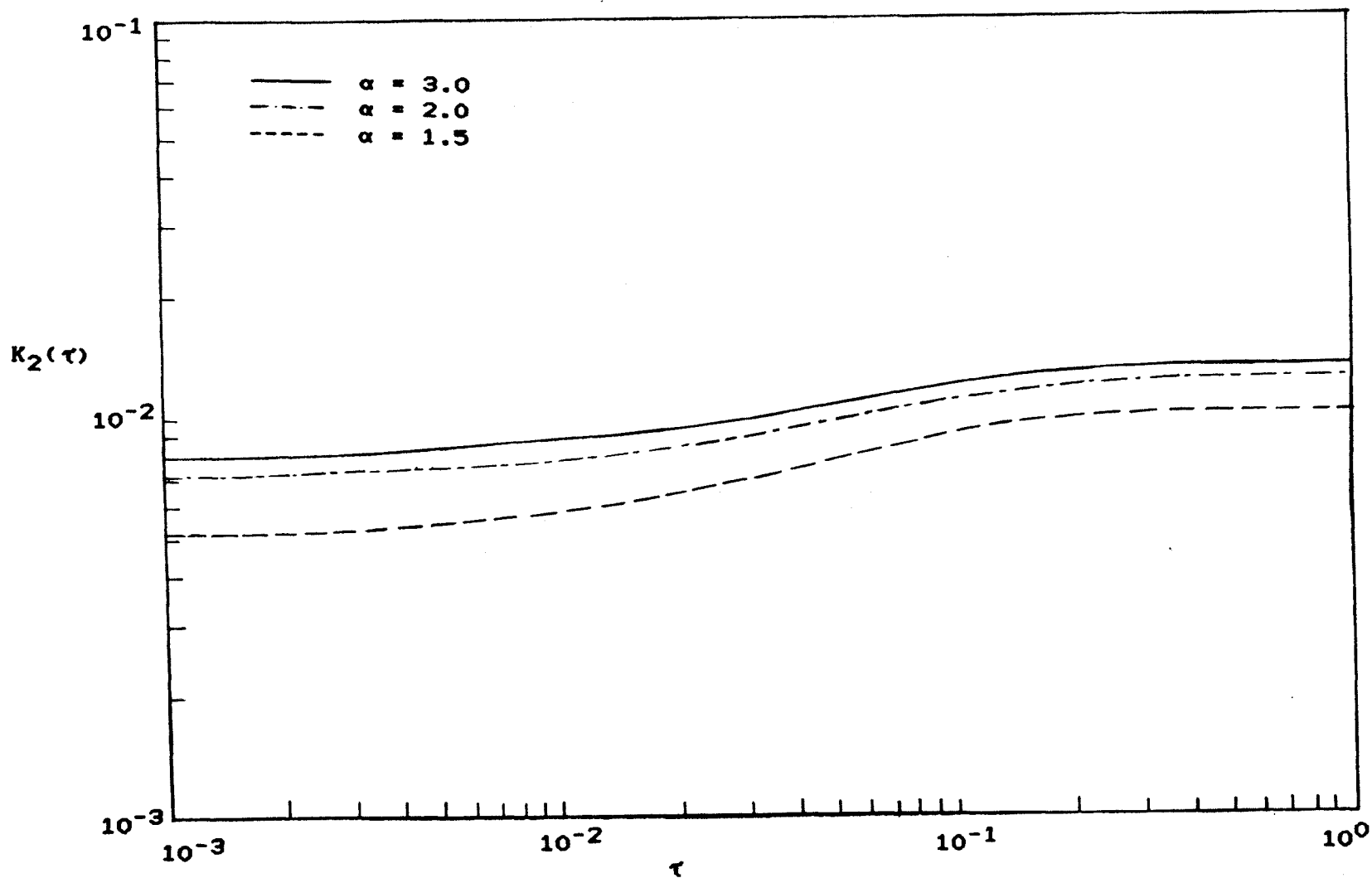


Fig. 11. Plot of $K_2(\tau)$ against dimensionless time τ under $P=0.1$ for three different set of polymers having the same τ_0 ($=1.48 \cdot 10^5$ NS/m²) and τ_y ($=3.29 \cdot 10^4$ N/m²)

$\tau=0.03$ whence K_2 is still exhibiting time-dependent behavior.

The set of value (K_2, Pe, τ) is chosen so as to compare the result obtained by Booras and Krantz. The purely convective cases are shown in Figure 14 and Figure 15.

It is interesting to observe in the purely convective case shown in Figures 14 and 15 that at low pressure gradient, the fluids exhibit a symmetrical mean concentration distribution about the point $X=0.015$ for pseudoplastic fluids and are skewed downstream at high pressure gradient due to the larger velocity (relative to the average velocity) near the axis of the tube. The pure convective solution for power-law fluids is also shown in Figures 14 and 15 for comparison. It is seen that as P increases the concentration distribution of Ellis fluids approaches that of power-law fluids.

Equation (86) gives the effect of molecular diffusion on the θ_n distribution for the appropriate value of α . The resulting θ_n shown in Figures 12 and 13 are symmetrical about

$$X = \frac{\tau}{V_0} \left(\frac{1}{2} V_{n1} + \frac{\alpha+1}{\alpha+3} V_{n2} \right)$$

It is seen that as P increases, the θ_n distributions shift downstream, approach the θ_n distribution of power-law fluid. This coincides with previous discussion that as P increases the fluids behave as power-law model. Also θ_n distribution shifts downstream as α increases for the same P . It may appear surprising that these θ_n curves exhibit nearly

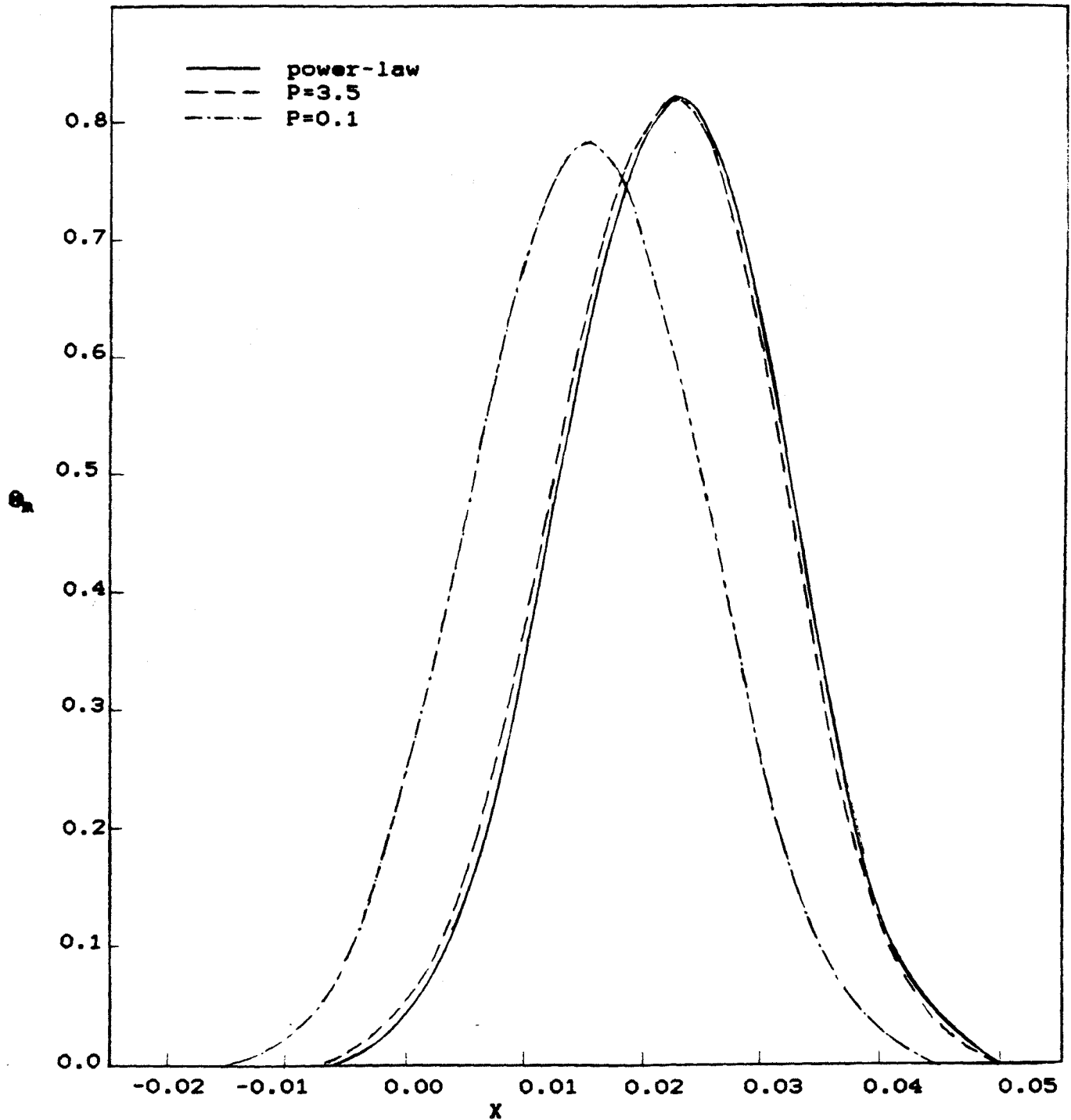


Fig. 12. Comparison of present solution (86) for the distribution θ_n against X of HIPS ($\alpha = 4.8$) at 463K with the result of the power-law fluid at $\tau=0.03$, and for $X_n=0.019$ and $Pe=1000$

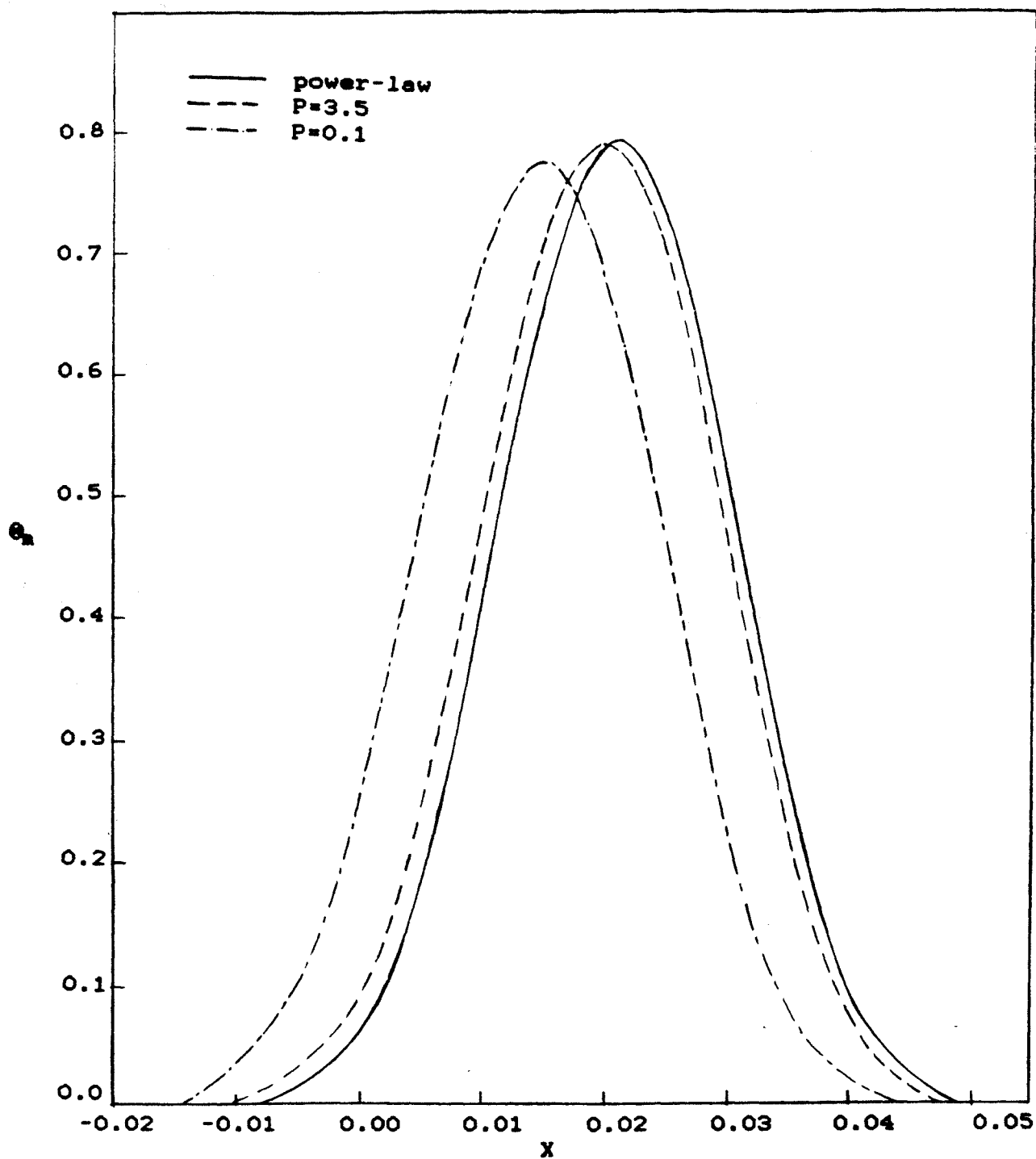


Fig. 13. Comparison of present solution (86) for the distribution θ_n against X of styrene acrylonitrile ($\alpha=3.59$) at 493K with result of the power-law fluid at $\tau=0.03$, and for $X_n=0.019$ and $Pe=1000$

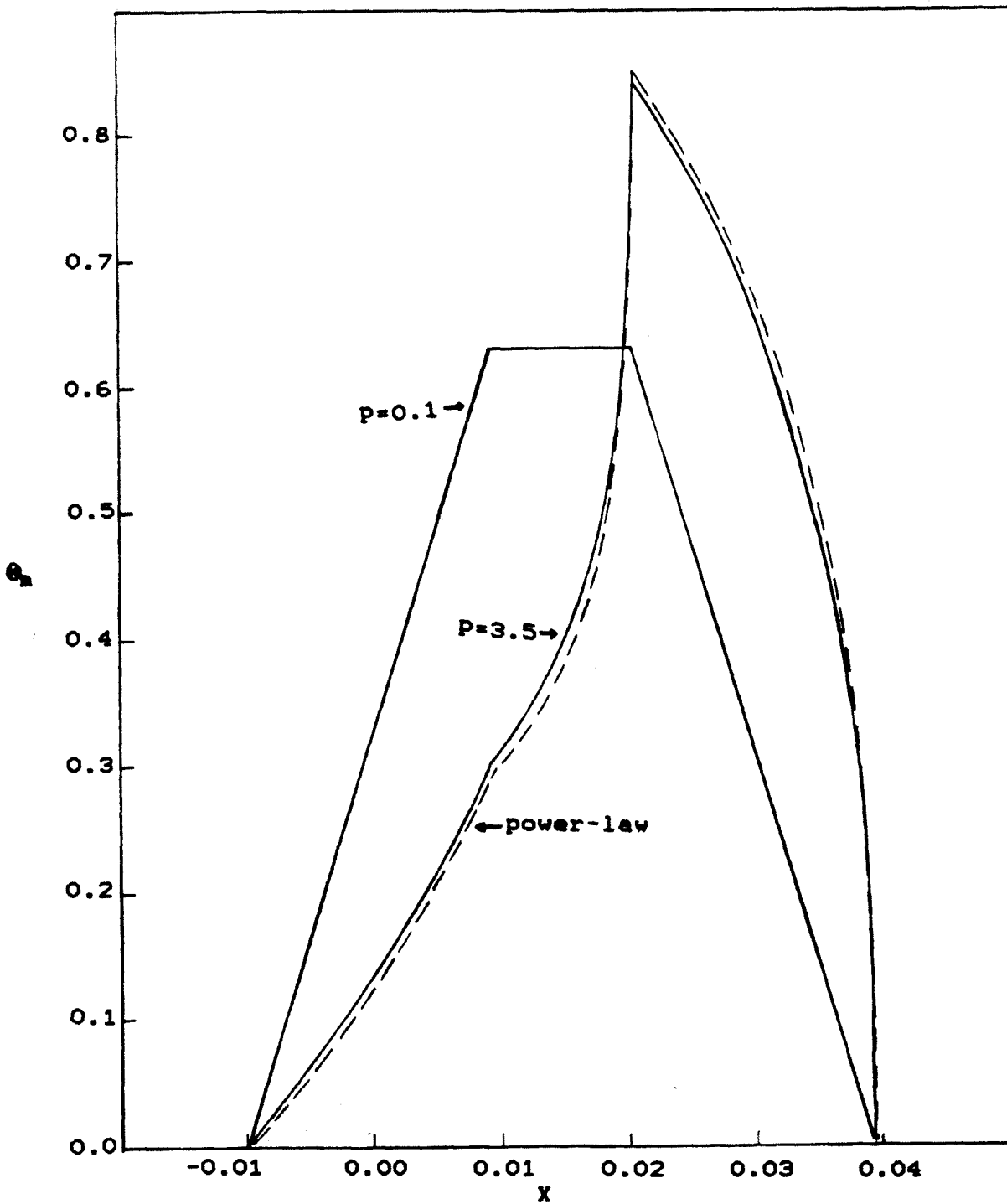


Fig. 14. Comparison of pure convective solution (40) for the distribution θ_p against X of HIPS ($\alpha = 4.8$) at 463K with the result of the power-law fluid at $\tau=0.03$, and for $X_p=0.019$ and $Pe=1000$

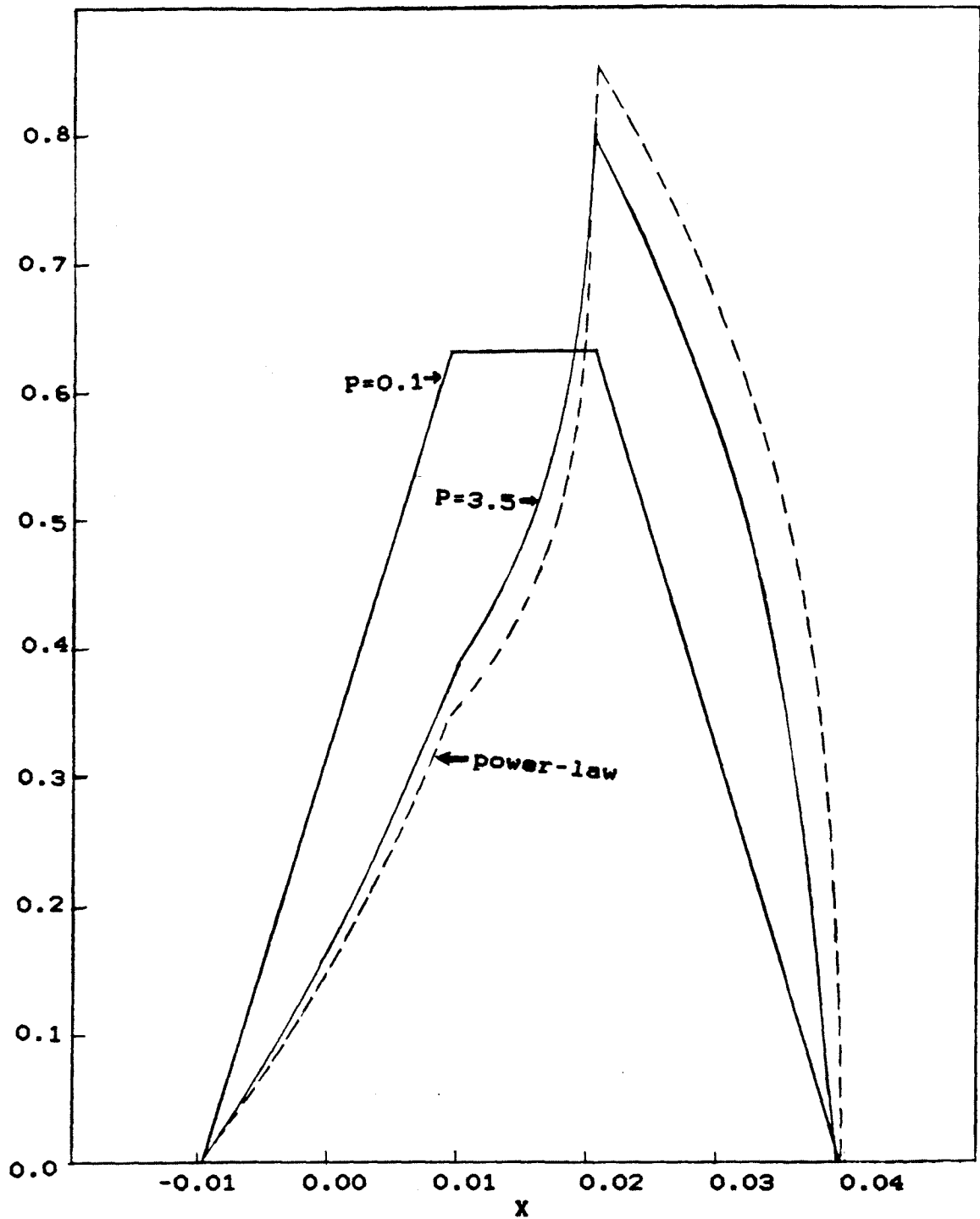


Fig. 15. Comparison of pure convective solution (40) for the distribution θ_s against X of styrene acrylonitrile ($\alpha=3.59$) at 493K with result of the power-law fluid at $\tau=0.03$, and for $X_s=0.019$ and $Pe=1000$

the same maximum at the same P , although the value of $K_2(\omega)$ for these two fluids differs considerably, i.e. at $P=2.5$ $K_2(\omega)-Pe^{-2}=3.812 \cdot 10^{-3}$ for $\alpha=4.8$, and $4.523 \cdot 10^{-3}$ for $\alpha=3.59$. This behavior arises because the time history of the two fluids is nearly identical; ζ determined from equation (87) at $\tau=0.03$ is nearly the same for both fluids.

These results for non-Newtonian Ellis model fluids illustrate quite dramatically the effect of molecular diffusion on the overall dispersion process. It seems quite remarkable that although the mean concentration distributions for purely convective dispersion are considerably unsymmetrical for non-Newtonian fluids under considerable shear stress the slightest amount of molecular diffusive action can render them symmetrical. The molecular diffusion smoothes out the distribution and this dispersing effect is enhanced by shear-thinning behaviour.

Here is a question as to whether the assumption that distribution θ_n is given by a purely diffusive process from time zero leading to equation (48) is valid for high Peclet number when the convective transport is large relative to the action of molecular diffusion. Note that this criticism of the generalized dispersion model restricts only to its applicability at the initial stages of the dispersion process. Certainly at larger values of τ our results and those of Gill and co-workers would appear to be applicable. Clearly more research is necessary to define the precise

limits of the generalized dispersion theory.

IV. CONCLUSIONS

It has been shown that an exact solution to the convective diffusion equation can be constructed by the generalized dispersion theory proposed by Gill (1967). This exact solution involves a dispersion model that includes third and higher order derivatives of mean concentration with respect to convected axis distance.

The effective dispersion coefficient, K_2 , is less sensitive to the flow index than K_2^* and for this reason it is a preferable definition of the dimensionless dispersion coefficient for Ellis model fluids. That is, moderately pseudoplastic fluids have dimensionless dispersion coefficients K_2 nearly equal to that of Newtonian fluids no matter how much the driving force P , is and hence can be treated as Newtonian fluids if the dispersion equation is appropriately nondimensionalized.

It is also seen that the dispersion coefficient depends on the driving force P . As P increases, the value of dispersion coefficient approaches the value of power law fluids. The results obtained by Booras and Krantz apply only to large driving force and can not predict the fluid behavior under low driving force. The usefulness of Ellis model is that it allows better prediction of dispersion for any value of the driving force P than would be possible with power-law model; and Ellis model shows clearly how non-Newtonian behaviour affects dispersion, particularly when the external

pressure gradient varies from low value to high value. Power-law model is not, straightly speaking, applicable to pipe flow of shear-thinning fluids. It is suggested that Ellis model is preferable to power-law model.

V. GLOSSARY

a	:	function defined by eq (7a)
\underline{a}	:	function defined by eq (28)
A	:	function defined by eq (51)
A_m	:	function defined by eq (72)
b	:	function defined by eq (7b)
B_{m1}	:	function defined by eq (75a)
B_{m2}	:	function defined by eq (75b)
C	:	local solute concentration
C_m	:	mean solute concentration
C_0	:	initial solute concentration
C^*	:	dimensionless concentration C/C_0
C_0	:	value of C^* at $r=0$
D	:	molecular diffusion coefficient
f_k	:	function defined by eq (45)
F_s	:	steady state solution of eq (62)
F_t	:	transit solution of eq (62)
g	:	function defined by eq (84b)
H	:	function defined by eq (89c)
$J_i(Z)$:	i^{th} -order Bessel function having argument Z
K	:	dispersion coefficient
K_i	:	generalized dispersion coefficient nondimensionalized with respect to V_0 and defined by eq (48)
K_i^*	:	generalized dispersion coefficient nondimensionalized with respect to V_x

K	:	function defined by eq (15)
K'	:	function defined by eq (29)
L	:	length of tube
n	:	flow behavior index
p	:	function defined by eq (16a)
P	:	function defined by eq (88)
Pe	:	Peclet number = RV_0/D
ΔP	:	pressure drop
q	:	function defined by equation (16b)
Q	:	volumetric flow rate
r	:	radial coordinate
R	:	radius of tube
t	:	time coordinate
\underline{t}	:	L/\bar{V}_x
T	:	transit time
v	:	function defined by eq (84a)
V_m	:	maximum velocity
\underline{V}_m	:	function defined by eq (32)
V_{m1}	:	function defined by eq (20a)
V_{m2}	:	function defined by eq (20b)
\underline{V}_{m1}	:	function defined by eq (30a)
\underline{V}_{m2}	:	function defined by eq (30b)
V_0	:	function defined by eq (30e)
V_x	:	local fluid velocity
\bar{V}_x	:	mean fluid velocity
x	:	axial coordinate

x_s	:	width of solute plug at time $t=0$
X	:	dimensionless axial coordinate Dx/R^2V_0 in a fixed coordinate system
X_1	:	dimensionless axial distance in coordinate system convected at mean fluid velocity
X_s	:	dimensionless width of solute plug Dx_s/R^2V_0
\underline{X}	:	axial distance in coordinate system convected at mean fluid velocity
y	:	dimensionless radial coordinate r/R
η	:	viscosity
η_1	:	dimensionless axial distance in coordinate system convected at mean fluid velocity
η_0	:	zero shear rate viscosity
η_{∞}	:	infinite shear rate viscosity
θ	:	dimensionless local concentration C/C_0
θ_m	:	dimensionless mean concentration
θ	:	dimensionless time
ξ	:	dimensionless radial coordinate r/R
ζ	:	function defined by eq (87)
α	:	flow behavior index
β	:	separation constant
τ	:	shear rate
τ	:	dimensionless time coordinate Dt/R^2
$\tau_{\frac{1}{2}}$:	value of shear stress at $\eta = \eta_0/2$
τ_0	:	empirical constant of Carreau model
τ_R	:	shear stress at wall
λ_n	:	eigenvalue

VI. APPENDIX

A. Program for equation (74)

```

#DEBUG
PROGRAM DISRERSION
IMPLICIT REAL*8(A-H,O-Z)
DOUBLE PRECISION N
DIMENSION XX(10),XXN(10)
OPEN(2,FILE='DISPER.XXX',STATUS='NEW')
OPEN(3,FILE='ALFA.DTA')
OPEN(4,FILE='DRIVE.DTA')
OPEN(5,FILE='EIGEN.VAL')
960 READ(3,920,END=930)N
WRITE(*,890)N
890 FORMAT(/' ALFA= ',D10.3)
REWIND 4
920 FORMAT(D4.1)
990 READ(4,920,END=940)P
WRITE(*,880)P
880 FORMAT(' T-R/T-.5 =',D10.4)
REWIND 5
IF (N-1.)790,780,790
780 G=0.DO
GO TO 781
790 G=2.*P***(N-1.)/(N+1.)
781 V1=1./(1.+G)
X1=V1*V1/192.
V2=G/(1.+G)
V22=(N+1.)*(N+11.)/(12.*(N+3.)*(N+5.)*(N+7.))
X2=V22*V1*V2
W=(N+1.)*(N+1.)/(2.*(N+5.)*(N+3.)*(N+3.)*(N+3.))
X3=W*V2*V2
WRITE(2,36)G,V1,V2,X1,X2,X3
36 FORMAT(///' H= ',D10.5/' V1= ',D10.5/' V2= ',D10.5
C/' X1= ',D10.5/' X2= ',D10.5/' X3= ',D10.5)
II=0
980 READ(5,950,END=970)XN,B0,B2,B3
WRITE(2,66)N,P,XN,B0,B2,B3
66 FORMAT(///' ALFA= ',D10.5/' D-P= ',D10.5/' XN= ',D10.5
C,' JO= ',D15.8,' J2= ',D10.5,' J3= ',D10.5/)
950 FORMAT(4D10.6)
II=II+1
BM=0.DO
XXN(II)=XN
A1=V1*B3/(XN*XN*XN*B0*B0)
A21=2.*V2/(B0*B0)
A22=B2/((N+3.)*XN*XN)
Y=0.
H=0.05

```

```

HH=3.14159/64.
SS=0.DO
UU=0.DO
TT=0.DO
VV=0.DO
TAU=0.0005
DO 4 J=1,100
IF (Y-1.)2,8,8
8 GO TO 10
2 Y=Y+H
SI=0.DO
C=0.DO
S=0.DO
T=0.DO
DO 5 I=1,100
IF(C-3.14159)17,7,7
7 GO TO 11
17 Z=XN*Y
C=C+HH
B1=Z*SIN(C)
S=S+4.*COS(B1)
C=C+HH
IF(C-3.14159)20,11,11
20 BB=Z*SIN(C)
T=T+2.*COS(BB)
5 CONTINUE
11 SI=(2.+S+T)/3.*HH/3.14159
SS=SS+4.*(Y**(N+4.))*SI
UU=UU+4.*(Y**(N+2.))*SI
Y=Y+H
IF (Y-1.)18,10,10
18 D=0.DO
S1=0.DO
T1=0.DO
SP=0.DO
DO 6 K=1,100
IF (D-3.14159)12,14,14
14 GO TO 15
12 Z1=XN*Y
D=D+HH
B5=Z1*SIN(D)
S1=S1+4.*COS(B5)
D=D+HH
IF (D-3.14159)9,15,15
9 B6=Z1*SIN(D)
T1=T1+2.*COS(B6)
6 CONTINUE
15 SP=(2.+S1+T1)/3.*HH/3.14159
TT=TT+2.*(Y**(N+4.))*SP
VV=VV+2.*(Y**(N+2.))*SP
4 CONTINUE
10 A11=(TT+SS+BO)*H/3./((N+3.)*(N+3.))
AN=A1+A21*(A22+A11)

```

```
BM1=V1*B2*AN/(XN*XN)
BX=(UU+VV+BO)*H/3.
BM2=(-1.)*V2*AN*BX/2.
BM=BM1+BM2
XX(II)=BM
WRITE(2,88)AN,BM1,BM2,BM
88  FORMAT(/' AN= ',D20.10/' BM1= ',D20.10/' BM2= '
C,D20.10/' BM= ',D20.10)
GOTO 980
970  DO 25 L=1,15
X4=0.DO
DO 26 JJ=1,II
Q=XXN(JJ)*XXN(JJ)*TAU*(-1.)
X4=4.*XX(JJ)*EXP(Q)+X4
26  CONTINUE
SU=X1+X2+X3-X4
WRITE(2,30)TAU,X4,SU
30  FORMAT(/' TAU= ',D20.10/' X4= ',D20.10/
C/' K2-1/PE**2= ',D20.10)
TAU=TAU*2.
25  CONTINUE
IF (N-1.)990,960,990
940  GOTO 960
930  STOP
END
```


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