CHAPTER 6

DISCUSSIONS

In this section the following items are discussed ;

1. The assumptions implied in the mathematical model .
2. The influence of controlled variables .
3. The prediction of axial dispersion coefficient .
4. Comparative analysis for experimental axial dispersion coefficient .

6.1 Assumptions implied in the mathematical model

The derivation of equation 2.6 involves various assumptions such as ;

1. The absence of radial gradients .
2. The existence of a uniform velocity profile .

6.1.1 Radial gradients

Although McHenry (8) mentioned that radial diffusivity is about sixfold less than axial diffusivity for turbulent flow of gases among particles , Smith et al (30) demonstrated that unusual radial velocity profiles can be encountered in the flow of gases through packed bed at every flow rate . They attributed these apparent anomalies to variation of void fraction with radial position in the packed bed . Smith indicated that radial variations of velocities exist in packed columns of various sizes and operating conditions . However large radial variations of velocities would be expected to result in a bed curve fitting between theoretical and experimental curves which is not the case as shown in appendix D .

A good fit between a theoretical curve to an experimental curve does not completely imply that there are no radial gradients . It may simply mean that the axial dispersion coefficient can describe whatever contribution radial gradients have on axial dispersion .

6.1.2 Velocity profile

Volkov et al (9) indicated that the fluctuation of the velocity field arised from the influence of packed bed parameter such as particle size distribution , mean particle size , the compaction method and the tube diameter . In case where the average particle sizes is large , where size distributions are wide , where particles are packed loosely , and where tube diameters are large , it has been found that interstitial velocity varies to some extent depending on the velocity measuring point within the bed . Otherwise the uniform velocity assumption can be valid .

6.2 Influence of controlled variables

The attention of this study is confined to the influence of three controlled variables on the axial dispersion phenomena , particle size , tube diameter and flow rate .

6.2.1 Particle size

The graphical representation shown in figure 5.1 , 5.2 , 5.3 , 5.4 and 5.5 infers that at a given tube diameter and a specified Reynolds number (or velocities for figure 5.5) , an increase in particle size gives rise to lesser axial dispersion . Volkov et al (9) presented a study for the elution of hydrogen by nitrogen in a 100 mm diameter tube and using three mean particle sizes of 0.36 , 0.52 and 0.75 mm as shown in figure 6.1 .

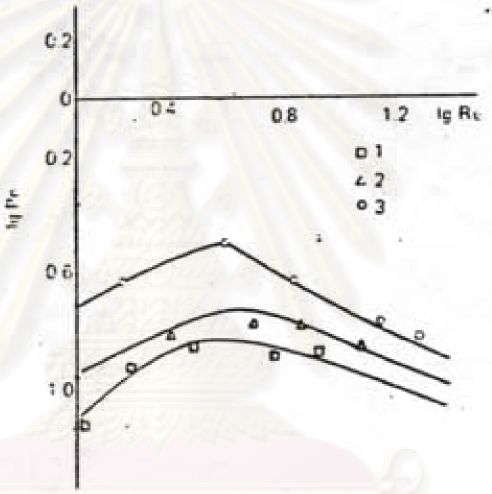

Fig. 6.1 Peclet numbers vs Reynolds numbers for d_p equal to 0.36 (1) , 0.52 (2) and 0.75 (3) .

Their result shows a similar particle size effect with that of this work . In contrast, the plots of $E_z(cm^2/s)$ versus d_p as in figure 6.2 using Hsu & Hyne's prediction shows a relationship opposite to that of ours . This controversial aspect reflects that the dispersion behaviour of small particle size does not obay the relationship given in equation 2.3 , especially , the particle size diameter term . Therefore some corrections are required to provide a more reliable prediction for small particles .

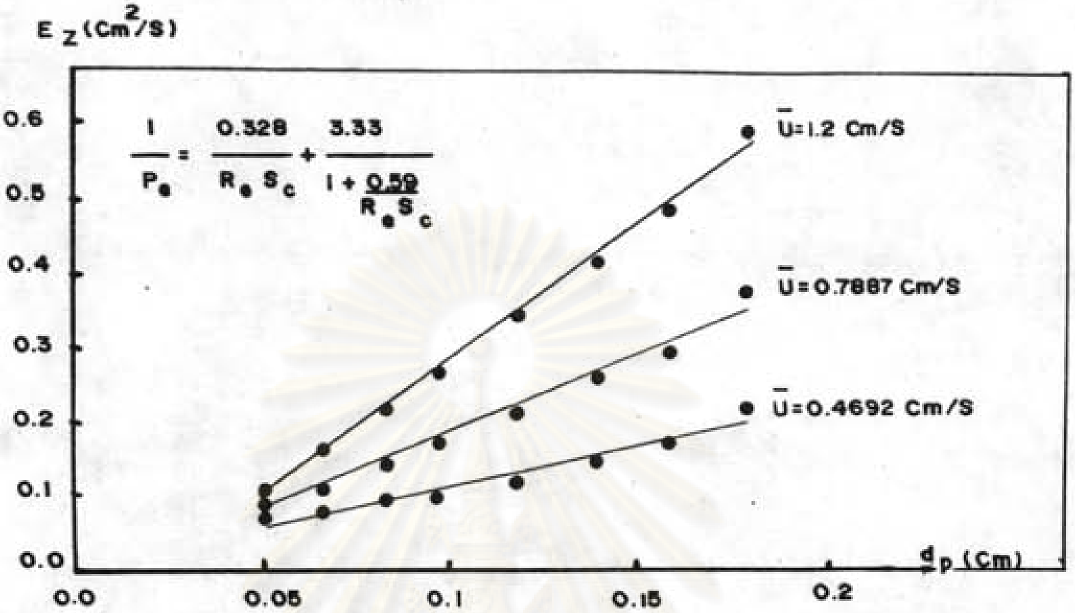

Fig. 6.2 Relationship between particle size and axial dispersion coefficientbased on Hsu & Hyne's equation .

6.2.2 Tube diameter

This study uses small diameter beds packed with very small sized particles ; data in the literature is generally devoted to larger diameter beds with particle sizes larger than those used in this study .

According to Gun's suggestion (20) , we selected tube to particle diameter ratios above ten so as to eliminate wall effects . In addition to ensure the elimination of end effects as suggested by Scott et al (34) , bed length to particle diameter ratios larger than 50 were also used in this study .

Figures 5.6 , 5.7 , 5.8 , 5.9 and 5.10 indicated effects of variations in tube diameter . As smaller bed diameter are used , the lesser the axial dispersion .

6.2.3 Flow rate

Since velocity is directly proportional to flow rate , so figure 5.11 presents the effect of flow rate upon axial dispersion . We find that increasing velocity yields a greater dispersion . Hsu & Hyne (37) modified general equation 2.3 ($E_z = rD_m + 0.5*u*d_p$ or $1/Pe = r/(Re*Sc) + 0.5$) and with their constansts , the predicted curves are plotted as illustrated in figure 6.3 . A similar tendency of this predicted curve plotting in E_z against u confirms our results .

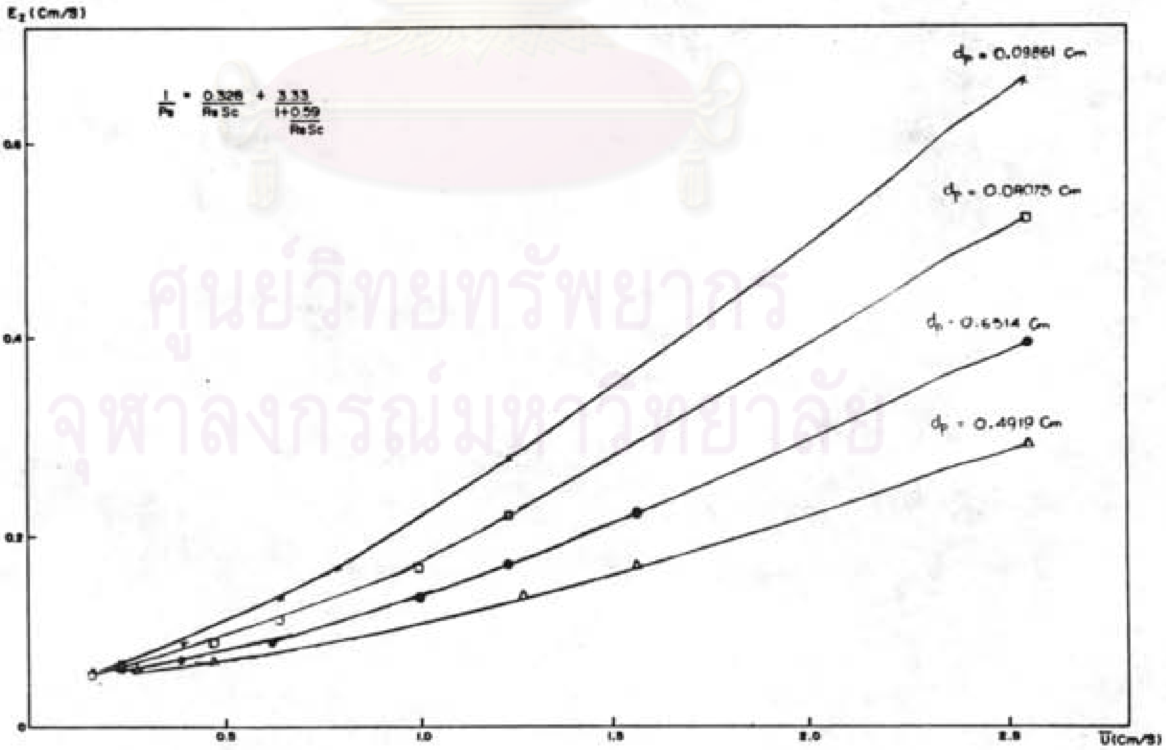

Fig. 6.3 Relationship between velocity and axial dispersion coefficient based on Hsu & Hyne's equation .

6.3 The prediction of axial dispersion coefficient

Since our experimental axial dispersion coefficient does not follow the relationship given in equation 2.3 . We hereby introduce a general power law to relate axial dispersion coefficient and the three factors discussed in the last section .

$$E_z/D_m = a(U)^b(d_p)^c(d_t)^d \qquad 6.1$$

All constants (a,b,c,d) will be evaluated by graphical methods using following equations :

$$\ln [E_z/D_m] = b\ln U + \ln [a(d_p)^c(d_t)^d] \qquad 6.2$$

$$\ln [E_z/D_m] = c\ln d_p + \ln [a(U)^b(d_t)^d] \qquad 6.3$$

$$\ln [E_z/D_m] = d\ln d_t + \ln [a(U)^b(d_p)^c \qquad 6.4$$

The logarithmic plot of E_z (cm^2/s) VS u (cm/s) as shown in figure 6.4 yields points scattering around a linear regression . A similar scatter arises from the other two plots (E_z versus d_p and E_z versus d_t) as shown in figures 6.5 and 6.6 , respectively . The slopes of these regressions equal to constants b , c and d . Constant a can be obtained by optimization using the following criteria

$$\varepsilon = 1/n \sum [E_z(\text{experimental}) - E_z(\text{predicted})]^2$$

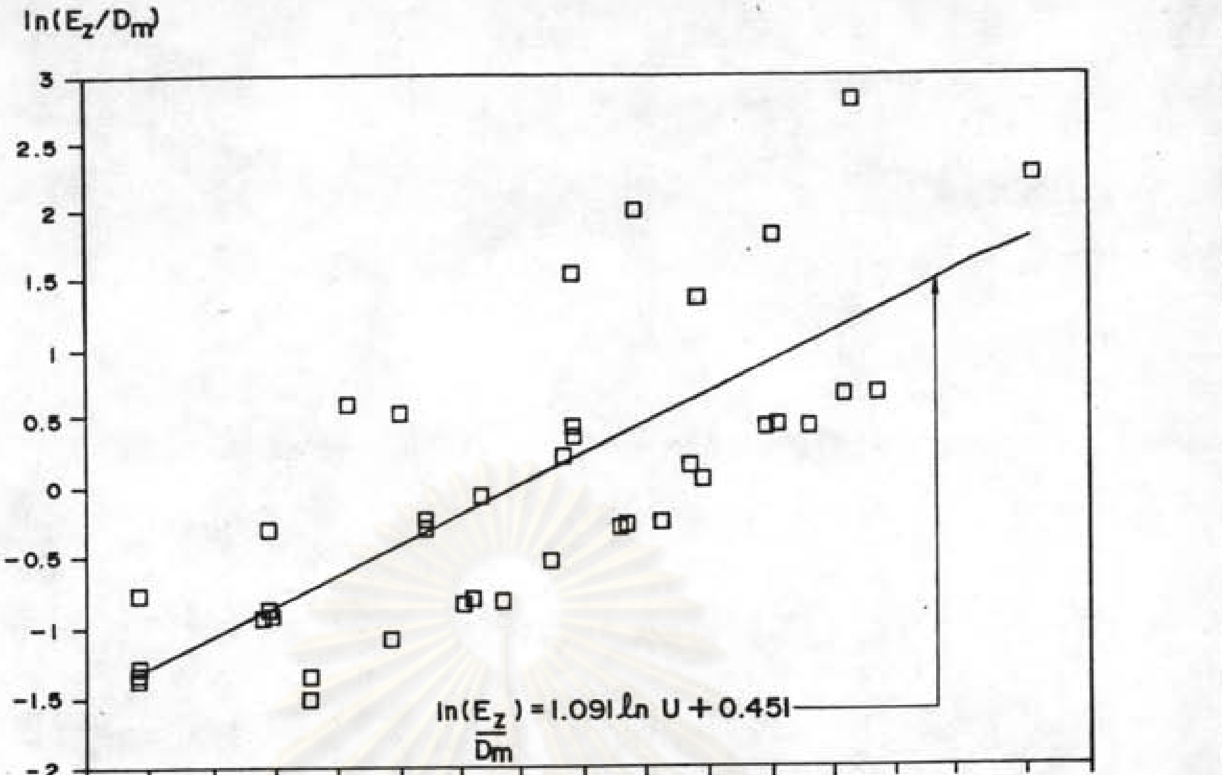

Fig. 6.4 Axial dispersion coefficient vs velocity for entire set of data showing linear regression line .

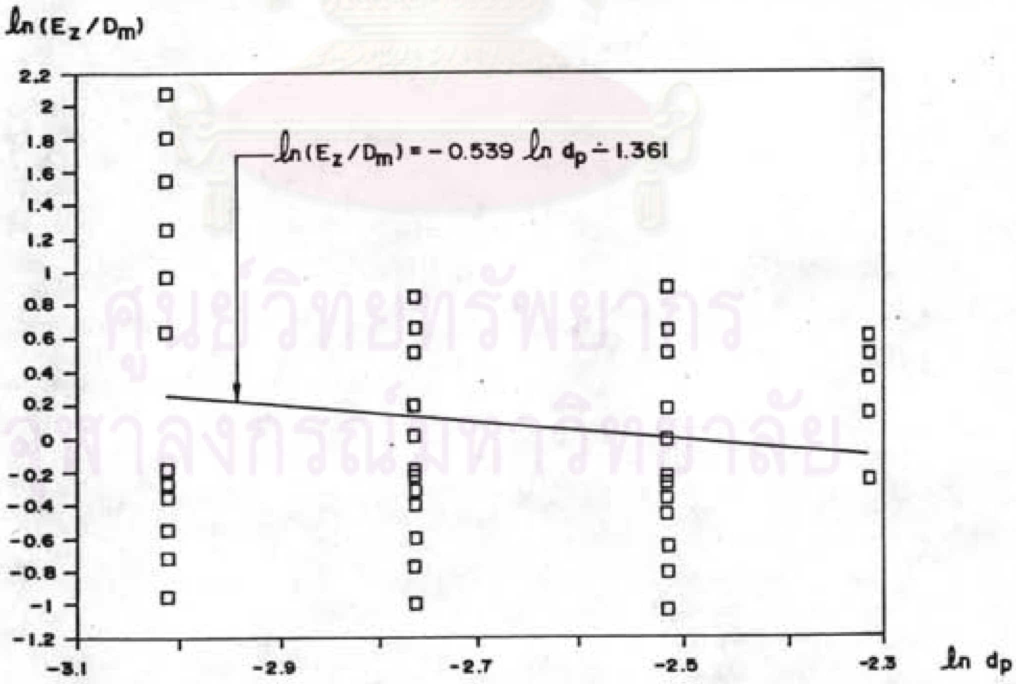

Fig. 6.5 Axial dispersion coefficient vs particle size for entire set of data at same fixed velocities showing linear regression line .

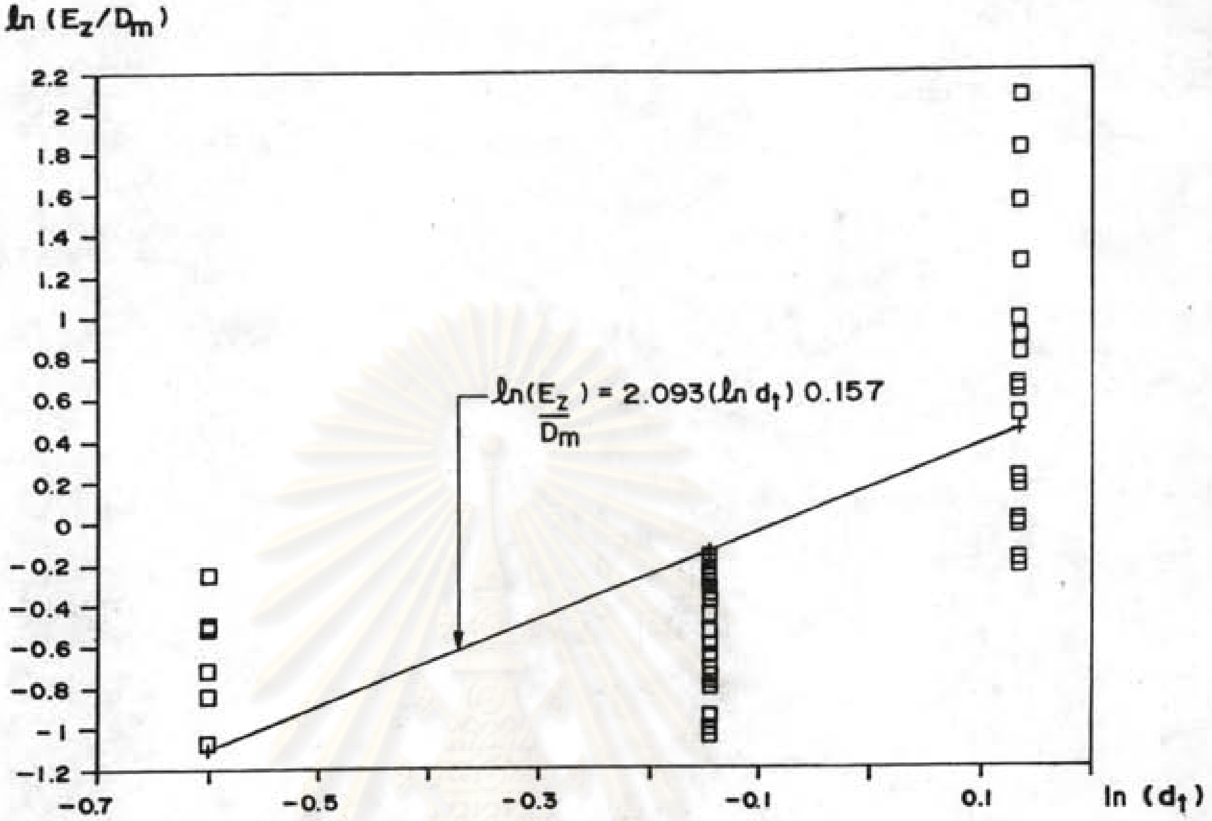

Fig. 6.6 Axial dispersion coefficient vs tube diameter for entire set of data at some fixed velocities showing linear regression line .

The optimization curve is given in figure 6.7 by plotting against a . Eventually , we get the relationship for predicting the axial dispersion coefficient as

$$E_z = 2.757(U)^{1.188}(d_p)^{-0.478}(d_t)^{1.921}(D_m) \qquad 6.5$$

Figure 6.8 depicts the graphical comparison between experimental dispersion coefficient and the predicted dispersion coefficient based on equation 6.5 .

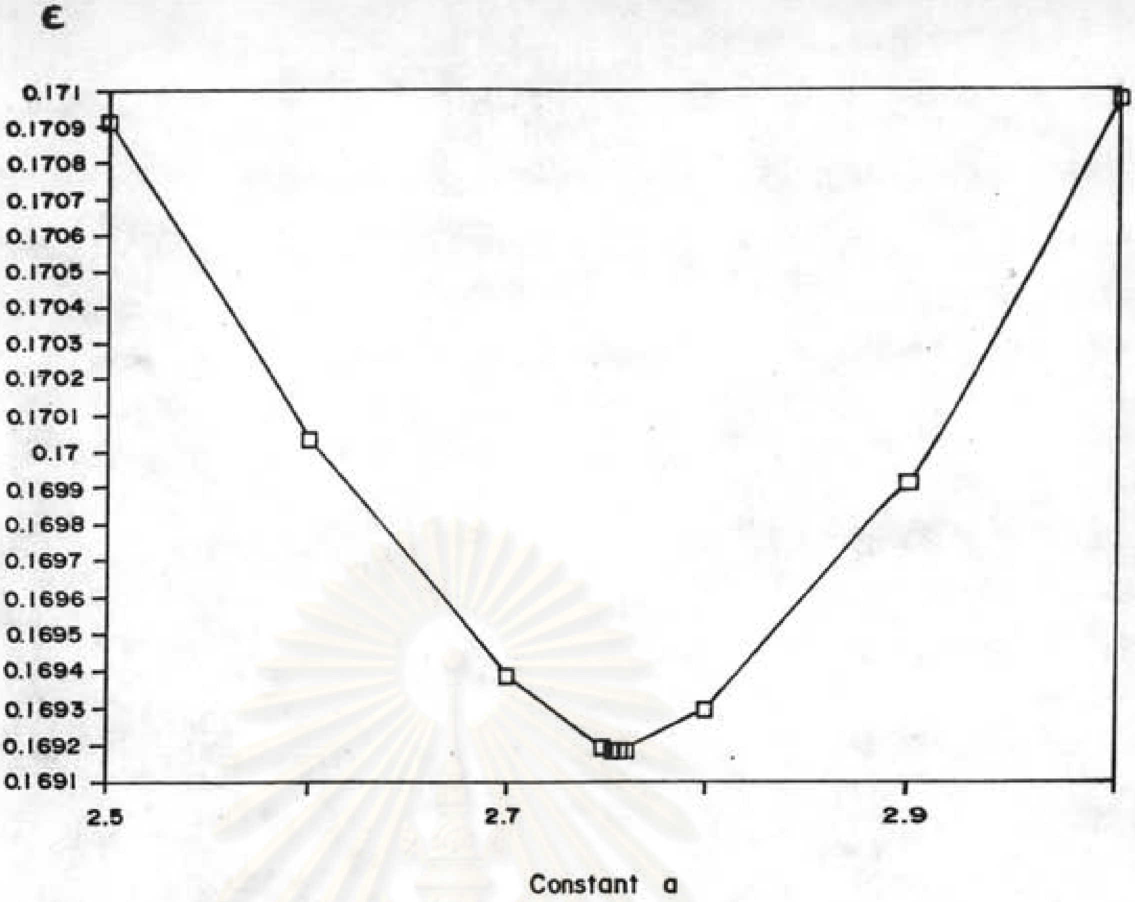

Fig. 6.7 Average minimal deviation of theoretical axial dispersion coefficient from experimental values versus constant a .

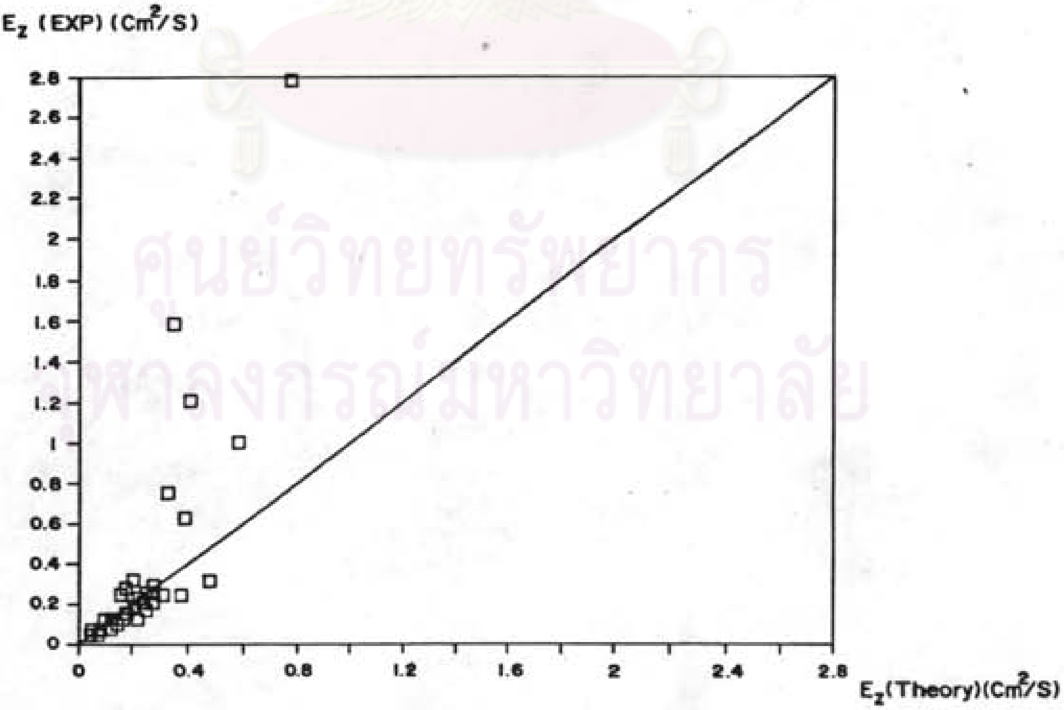

Fig. 6.8 Comparison of measured dispersion coefficient with that obtained with emperical formula .

6.4 Comparative analysis for experimental axial dispersion coefficient

As no propane - methane molecular diffusivity information was available , here is reported data for similar pairs of hydrocarbons as given in table 6.1

TABLE 6.1 DIFFUSION COEFFICIENTS IN BINARY GAS SYSTEMS

$D_{12}P$ is the product of D in square centimeters per second and the pressure in atmospheres

System	T, °K	$D_{12}P$ (obs.)	$D_{12}P$ (calc. using force constants from viscosity)	Error, %*	$D_{12}P$ (calc. using estimated force)	Error, %*	$D_{12}P$ Arnold method	Error, %*	$D_{12}P$ Gilliland method	Error, %*	$D_{12}P$ Slattery method	Error, %*
Ethane-methane	293	0.0850	0.079	−7	0.0811	−5	0.0935	+10	0.098	+15	0.152	−7
Ethane-propane	293	0.163	0.157	−4	0.167	+2	0.162	−1	0.143	−12	0.098	+15

* % error = (calculated − experimental)/experimental × 100

Source : The properties of Gases and Liquids , Reid , pp.275

axial dispersion coefficients (E_z) obtained for Reynolds numbers between 0.14 - 1.50 as shown in table 5.2 indicate the same order of magnitude as molecular diffusion coefficient (D_m) of the ethane - propane system . This shows that our experimental axial dispersion coefficients (E_z) are very small and probably can be neglected for engineering purposes .

8/ See all formula of calculated methods shown in table 6.1 in reference no. 36